# The Impact of Artificial Intelligence on Materials Engineering Research

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Major Qualifying Project

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# **Abstract**

Materials engineering is an ever-expanding field with broad applications, and Artificial Intelligence (AI) shows great promise for advancing new materials. While previous research has focused on developing new materials, little research has explored the potential of AI in assisting materials engineers, engineer-AI interactions, and its incorporation into decision-making processes. To address this issue, we devised a rubric to assess various AI systems currently on the market based on specific criteria relevant for engineers' decision-making (e.g. ease of use, trustworthiness, memory, accuracy, and speed). We independently applied this rubric to evaluate eight AI systems: ChatGPT, Elicit, SciSpace Copilot, Writeful X, Paperpal, QuillBot, PaperDigest, and Notion. We then incorporated the rubric into a survey distributed to materials engineers, who provided ratings about their perceptions, decision-making processes, and overall evaluations of these eight systems. Finally, we conducted a case study where an engineering student used AI to write an academic paper on a quaternary alloy system, documenting their firsthand experience and perceptions of AI in materials science. Overall, this study is among the first to provide insights into AI's potential applications and implications in materials engineering.

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The field of materials engineering is constantly evolving, driven by the quest to develop new materials with enhanced properties for various applications, such as the creation of the ternary CrCoNi system which has been extensively studied because of its unique mechanical properties, exhibiting higher strength and ductility than quaternary or quinary alloys made from this system (Ding et al., 2022; Laplanche et al., 2017; Miao et al., 2017). In recent years, the field of Artificial Intelligence (AI) has emerged as a powerful tool with the potential to revolutionize and create new possibilities for various industries, including materials engineering. Leveraging AI can significantly expedite the development process, enabling engineers to make informed decisions. However, to harness the full potential of AI in this domain, it is crucial to understand how materials engineers can effectively integrate and interact with AI systems as they identify key properties of new candidate materials. While previous research has focused on materials development, little attention has been given to exploring the potential of AI in assisting engineers in this area. Additionally, there is a scarcity of research concerning the interaction between engineers and AI, particularly within the domain of materials engineering. Furthermore, the incorporation of AI in decision-making processes within this field remains largely unexplored.

AI is a revolutionary technology that has gained significant attention since its inception in 1955. Coined by John McCarthy, AI is defined as "the science and engineering of making intelligent machines" (Manning, 2020). Additionally, AI has been studied by authors Stuart Russell and Peter Norvig, who published *Artificial Intelligence: A Modern Approach*, which is one of the leading textbooks in the study of AI. Russell and Norvig categorize AI into four goals on the basis of rationality and thinking vs acting: systems that exhibit human-like thinking, systems that imitate human behavior, systems that think rationally, and systems that act rationally (*What Is Artificial Intelligence (AI)?*, n.d.). AI contains two subcategories: machine learning

(ML) and deep learning. Machine learning focuses on enhancing computer agents' perception, knowledge, thinking, or actions through training with vast datasets; while deep learning employs neural networks to simulate human brain behavior, enabling learning from datasets and generating language (Manning, 2020) (*What Is Deep Learning?*, n.d.). Finally, AI encompasses two primary types: weak AI and strong AI. Weak AI, also referred to as Narrow AI or Artificial Narrow Intelligence (ANI), is designed to perform specific tasks. On the other hand, Strong AI includes Artificial General Intelligence (AGI), which possesses intelligence comparable to humans, and Artificial Super Intelligence (ASI), which surpasses human intelligence (*What Is Artificial Intelligence (AI)?*, n.d.). In this paper, we analyzed Chatbox AI systems, which have a limited memory and are restricted to a single medium (text-based chat), classifying them and similar systems as a form of Narrow or Weak AI (Cashman, 2023).

The primary goal of the present study was to investigate how materials engineers can leverage AI to facilitate the development of new materials. To achieve this objective, we adopted a comprehensive approach, as we established evaluative criteria for popular AI systems, characterized engineers' perceptions and attitudes towards these systems, and explored decision-making processes within the context of AI integration. To evaluate AI systems, we devised a rubric that assessed various AI systems based on specific criteria. This rubric served as a foundation for a survey designed to gather insights from materials engineers. The survey encompassed a diverse range of question types, exploring general perceptions and attitudes towards AI, as well as engineers' evaluations of eight prominent AI systems using the established rubric. Furthermore, the survey aimed to understand if materials engineers trust AI and if it can be implemented into their decision-making processes. Finally, to provide real-world insights on the practical application of AI in materials science, we conducted a case study where

an engineer utilized AI to write an academic paper on a system containing four elements, a quaternary alloy.

Through this comprehensive approach, encompassing rubric-based evaluations, surveys, and a case study, this study sought to shed light on the untapped potential of the utility of AI in materials engineering. By identifying the strengths and limitations of AI systems and understanding how materials engineers interact with AI, we aimed to pave the way for a more efficient and productive future in materials engineering. This project addressed a critical gap in the current research landscape and aimed to contribute to the advancement of materials science and provide valuable guidance for future applications of AI in all engineering contexts.

# What is Artificial Intelligence

Artificial Intelligence (AI) is a term coined by the emeritus Stanford Professor John McCarthy in 1955. He defined it as "the science and engineering of making intelligent machines" (Manning, 2020). Additionally, AI has been studied by authors Stuart Russell and Peter Norvig, who published *Artificial Intelligence: A Modern Approach*, which is one of the leading textbooks in the study of AI. Russell and Norvig categorize AI into four goals on the basis of rationality and thinking vs acting: systems that exhibit human-like thinking, systems that imitate human behavior, systems that think rationally, and systems that act rationally (*What Is Artificial Intelligence (AI)?*, n.d.). Based on this research, AI is a multidisciplinary field that combines computer science and robust datasets to enable problem-solving (*What Is Artificial Intelligence (AI)?*, n.d.). Two notable subcategories of AI include (1) machine learning (ML), which focuses on how computer agents can enhance their perception, knowledge, thinking, or actions via training with large amounts of data, and (2) deep learning, is comprised of a neural

network that attempts to simulate the behavior of the human brain, allowing it to learn from large amounts of data (Manning, 2020) (*What Is Deep Learning?*, n.d.).

Artificial Intelligence encompasses two primary types: weak AI and strong AI. Weak AI, also referred to as Narrow AI or Artificial Narrow Intelligence (ANI), is designed to perform specific tasks. For instance, autonomous vehicles are designed only to drive safely, while Apple's Siri or Amazon's Alexa can only perform tasks when prompted and connected to other smart devices. While these AI systems demonstrate intelligence, their capabilities are confined to specific domains, hence the term Narrow AI, as they cannot venture into other fields. On the other hand, Strong AI includes Artificial General Intelligence (AGI), which possesses intelligence comparable to humans, and Artificial Super Intelligence (ASI), which surpasses human intelligence (What Is Artificial Intelligence (AI)?, n.d.). Chatbot AI systems, such as Chat Generative Pre-Trained Transformer (ChatGPT), employ natural language processing (NLP) models that draw upon very large corpuses of text data to learn the statistical patterns and regularities of the human language, in order to generate words and sentences that mirror conversation in human dialogue (Paul et al., 2023). Chatbox AI systems have a limited memory and since they are restricted to a single medium (text-based chat), it classifies them and similar systems as a form of Narrow or Weak AI (Cashman, 2023). ChatGPT and similar AI systems find applications in speech recognition, customer service, computer vision, recommendation engines, automated stock trading, and other domains (What Is Artificial Intelligence (AI)?, n.d.).

Despite the aforementioned benefits, there are potential drawbacks associated with AI systems. Users may become overly reliant on AI for decision-making, chatbot AI systems can generate misinformation that is not based on facts, and the systems may exhibit bias and discriminatory behavior in the text generated, due to biases in the data that the AI was trained on.

In addition, chatbox AI systems may collect and store data from user interactions, there may be a lack of contextual understanding when providing responses, the AI may influence users' moral judgments, and the systems may even be exploited for generating phishing emails and facilitating attacks (Paul et al., 2023). Nevertheless, AI systems like ChatGPT can be especially useful for engineers in various tasks, such as design assistance, cost estimating, rendering and visualization, code compliance, energy analysis, note-taking, email composition, research, and code generation (ArchSmarter, 2023). These AI systems can help save time and increase the productivity of engineers, however, it is important to note that they still rely on human decision-making, which cannot be completely substituted by AI.

# **Information Processing and Decision-Making in Engineering Contexts**

# Information Processing

Cognitive psychologists use the information processing model to explain how humans receive, process, and utilize information (Borris, 2022). One of the major information processing models, the Baddeley-Hitch model, as known as the "working model," suggests that short-term memory has several subsystems that process different types of information. These include the (1) phonological loop, which processes auditory information, (2) the visuospatial sketchpad, which processes visual information, (3) the central executive, which coordinates information processing, making decisions, critical thinking, and controlling attention, and (4) the episodic buffer, which temporarily stores information from the other parts of the model (Borris, 2022).

Engineers rely on all these subsystems to effectively process information and make informed decisions. For instance, engineers utilize the phonological loop to process auditory information received from colleagues, while they employ the visuospatial sketchpad to analyze

visual data, such as when interacting with machines to identify potential issues. Moreover, the visuospatial sketchpad also plays a crucial role in interpreting the additional layer of information provided by AI. Meanwhile, the central executive plays a key role in interpreting the diverse input of information to aid engineers in decision-making, while the episodic buffer temporarily stores all the information involved in the process. However, the information processing model relies on several fundamental assumptions, such as its capacity to manage and process information, the requirement of a controlled system, and the brain's limited memory capacity (Borris, 2022).

#### Information Processing in Decision-Making

Decisions arise from the dynamic interplay of multiple functional systems, working in parallel to process information in distinct ways. The process of decision-making involves three primary action-selection components: the Pavlovian system, the habit system, and the deliberative system.

The Pavlovian system triggers an action from a limited set of potential actions in response to specific stimuli. Conversely, the habit system allows for arbitrary stimulus-action pairings, enabling automatic and ingrained behaviors. The deliberative system, characterized by flexibility, utilizes knowledge of the causal structure of the world to envision future scenarios, facilitating the planning of actions that optimize expected rewards. Each of these systems involves various anatomical structures that contribute to their information processing.

The hippocampus, for instance, plays a crucial role in creating a mental map of the world, allowing for the exploration and imagination of future possibilities. The dorsal striatal neurons contribute to forming associations between situations and corresponding actions. Furthermore,

the ventral striatum serves to maintain representations of value across all three systems, contributing to the decision-making processes (van der Meer et al., 2012).

As previously mentioned, engineers encounter numerous decisions, and they must utilize all three primary action-selection components. For instance, the Pavlovian system allows engineers to swiftly react to an alarm in order to resolve a problem safely, which is especially important for engineers working on a chemical plant or in a high-risk environment. The habit system allows engineers quickly to inspect product quality by leveraging their accumulated experience with specific dimensions, specifications, and performance indicators. On the other hand, the deliberative system allows engineers to plan for future endeavors, whether it involves designing a new machine or carefully weighing potential solutions to a problem, in order to make a sound decision.

In the realm of materials engineers, the Pavlovian system plays a pivotal role in facilitating a cyclical process of testing, analyzing, and refining designs. Materials engineers employ this system to learn from past experiments, making necessary adjustments to optimize the performance and properties of materials. Moreover, by leveraging their accumulated knowledge and expertise, engineers utilize the habit system to expedite the discovery of new materials. Their familiarity with specific dimensions, specifications, and performance indicators enables them to swiftly assess product quality and make informed decisions. Additionally, materials engineers employ the deliberative system to strategically test various alloys, efficiently identifying optimal solutions for specific applications. They plan meticulously for future material usage, considering factors such as durability, cost-effectiveness, and performance requirements. By integrating these three primary action-selection components, materials engineers enhance

their decision-making processes, thereby ensuring the development of innovative and functional materials tailored to diverse industry needs.

#### **Decision-Making Theories**

Decision-making is a fundamental yet complex psychological process that individuals engage in on a daily basis. A decision represents an ill-structured problem involving evaluating multiple options and ultimately committing to a particular choice. There are different perspectives on decision-making: normative models propose that decisions aim to maximize utility, while naturalistic approaches suggest that personal beliefs and past experiences influence decision-making (Zhang, n.d.).

Normative models encompass various frameworks, such as rational choice models, cost-benefit analysis, and risk assessment models. Rational-choice models involve identifying options, establishing evaluation criteria, weighing each option, and selecting the one with the highest score. The cost-benefit analysis attempts to quantify values associated with each decision, while the risk assessment model incorporates probability analysis to evaluate expected values, taking into account the consequences of both false positives and false negatives (Zhang, n.d.).

Naturalistic approaches to decision-making include narrative-based decision-making, identify-based decision-making, and the influence of the unconscious mind on decision-making (Jonassen, 2012). These perspectives emphasize the role of personal experiences, beliefs, and psychological factors in shaping decision-making processes. The difference in the normative models and naturalists approaches may cause an interesting tension for an experienced engineer when making decisions. On one hand, they may "trust their gut" and use their accumulated knowledge to make a decision (naturalistic approach), or on the other hand they may choose an

optimal solution proposed by AI and supported by rational-choice models, that may ignore or disregard some factor or variable (normative model).

Decisions are typically made under three circumstances: risk, uncertainty, and ambiguity. Risk refers to situations where the probabilities of different outcomes are known. Uncertainty arises when the probabilities of outcomes are unknown or difficult to estimate accurately. Ambiguity occurs when the goals, options, or outcomes are unclear or poorly defined (Zhang, n.d.).

Furthermore, decisions can be classified into four categories; choices (selection of a subset from a larger set of alternatives), acceptance/rejections (binary decisions), evaluations (assigning worth to an option), and constructions (attempting to create an ideal solution within available resources) (Zhang, n.d.). Engineers make decisions in all four categories and therefore must be well-equipped to solve any problem. Overall, decision-making can be understood through various theories and models that consider rationality, value assessments, risk analysis, and the influence of personal experiences and beliefs.

# Steps for Decision-Making

The typical engineering decision-making process, as defined by the Brown University Division of Engineering, involves several steps. First, it is crucial to clearly define the objective of solving a specific problem. Next, all possible solutions are generated. Then, the predicted outcome of each solution is assessed. Finally, the best solution is determined by examining the pros and cons, and considering costs and benefits (Brown University, n.d.). Engineers commonly adhere to this systematic approach when making decisions, however, the integration of AI introduces additional layers of information that must be processed and taken into account to make well-informed decisions.

David Ullman, a professor, author, and specialist on product design and decision-making, outlines his twelve-step approach to decision-making (Ullman, 2010); (Zhang, n.d.). These steps are as follows:

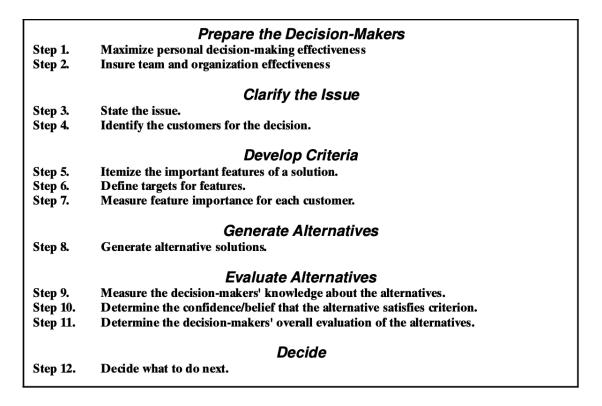


Figure 1. David Ullman's twelve-step approach to decision-making. This figure was taken directly from Ullman's paper (Ullman, 2010).

When making decisions, engineers have a responsibility to consider the impact on both their company and consumers. They must take into account various factors, including budgetary constraints and project timelines, which complicate the decisions even more. By following these steps, decision-makers can effectively approach the decision-making process, ensuring thorough evaluation of alternatives and considering important criteria for reaching the best possible solution.

#### **Problem-Solving**

Decision-making is the most common kind of problem-solving (Jonassen, 2012). Each problem possesses a unique context, demanding specific skills to resolve it, and engineers must be prepared to solve each distinctive problem. The complexity of a problem can be influenced by various external factors, including cultural, organizational, and social contexts, the level of difficulty and knowledge required, the problem's structure, the problem-solver's perspective, and whether the problem is static or dynamic.

Problem-solving can be delineated into five phases: identification, information searching, solution identification, solution evaluation, and monitoring. Additionally, it is crucial to acknowledge the degree of structuredness inherent in a problem, which can range from ill-structured to well-structured. Well-structured problems provide all the necessary information for their resolution, requiring a limited number of rules and principles, and featuring clear and comprehensible solutions. Well-structured problems are not typically found in everyday work for engineers, however they are found in formal educational contexts, like the practice problems found at the end of textbooks. Conversely, ill-structured problems lack self-contained boundaries, their solutions are unpredictable, they often involve interdisciplinary aspects and conflicting goals, and multiple solutions may exist. These problems are encountered more frequently in everyday life and work, for example, an engineer may need to come up with a solution to fix a machine in which the problem is unknown and there are no boundaries to the solution (Jonassen, 2015).

#### Tools to Make Decisions

The tools to aid decision-making can be categorized into rational choice tools and narrative methods. One rational choice tool is the decision matrix, also known as the Pugh

method. It involves representing options in rows and criteria, assessed through quantitative or qualitative values, in columns within a matrix or table. Another rational choice tool is the SWOT analysis, which evaluates both internal and external forces, encompassing strengths, weaknesses, opportunities, and threats associated with a decision. Force-field analysis is yet another rational choice tool that examines the forces supporting or opposing a specific action, considering the pros and cons. Lastly, argumentation serves as a rational choice tool where decision-makers generate arguments to resolve conflicts among competing options. These tools allow engineers to logically weigh potential options while considering all external factors.

Narrative methods offer alternative approaches to decision-making. Hypothetical scenarios are created, constructing stories that anticipate future events during times of uncertainty. Mental simulations represent another narrative method, involving the formation of scenarios that explain how events have unfolded from the past to the present and how they are likely to progress in the future, drawing upon past experiences. Narrative methods allow engineers to work through the outcome(s) of potential options. The tools from both categories rely on the assumptions made regarding the situation and assist individuals in offloading cognitive responsibility when making judgments (Jonassen, 2012). When using these tools, AI can contribute to the generation of the tools or even consider other factors or outcomes that the engineer may not have already examined.

#### **How Engineers Solve Problems and Interact with AI**

Engineers are trained to approach problems with a pragmatic and logical mindset, prioritizing efficiency, utility, and cost minimization over aesthetics and flair (Zhang, n.d.). The problems they encounter vary in terms of their structuredness, encompassing algorithms,

troubleshooting, strategic performance issues, and planning problems. The three common kinds of problems that engineers solve are decision-making, troubleshooting, and design problems. Decision-making problems often require engineers to select the most suitable solution, address an issue, or determine a course of action. Rational-choice tools like decision matrices and narrative methods are commonly employed to solve such problems. However, these problems are rarely content-neutral, as the decision-maker's beliefs and knowledge may influence the decision-making process. Troubleshooting problems arise when a system is not functioning properly. Engineers rely on the symptoms to generate and test hypotheses about potential faults. Design problems are typically ill-defined, featuring ambiguous goals and multiple potential solutions. To solve these types of problems, engineers define the problem, develop a conceptual design, and proceed with preliminary, detailed, and final designs (Jonassen, 2015).

When engineers interact with AI, there are three essential elements in the interaction: the user, the system, and the context (Chen et al., 2021). In order for engineers to successfully use AI and enhance their productivity, the explainability of the AI systems' behavior becomes crucial. It should be considered from three different dimensions: the intended recipient of the explanation, the purpose for which the explanation is needed, and the contextual factors and other relevant information associated with the explanation (Ferreira & Monteiro, 2020). By incorporating these dimensions, AI explanations can be tailored to fit the engineer's specific needs and expectations in the right format and at the appropriate moment. The integration of these three elements acknowledges the impact of the user's internal state (such as predispositions, expectations, needs, motivation, and mood), the characteristics of the designed system (such as complexity, purpose, usability, and functionality), and the context in which the

interaction occurs (including organizational and social settings, the meaningfulness of the activity, and voluntariness of use) (Chen et al., 2021).

Explainability plays a vital role in this context, as engineers require more than just the output of the AI model. Explanations cannot be standardized since each engineer seeks explanations based on their unique expectations, background, and needs. However, eXplainable AI (XAI) is just one element and must be complemented by other data to have meaningful implications for engineers in problem-solving and decision-making processes. XAI is critical across all domains utilizing AI, as a proper understanding of the user (engineer) is essential to provide adequate explanations that enhance their productivity (Ferreira & Monteiro, 2020).

## **AI Systems**

AI systems encompass a wide range of functions, depending on the user's goals. Eight AI systems (ChatGPT, Elicit, SciSpace Copilot, Writefull X, Paperpal, QuillBot, Paper Digest, and Notion) can be separated into three categories based on their functionalities: interactive response generation (e.g. ChatGPT), research support and analysis (e.g. Elicit, SciSpace Copilot, Writefull X, and Paper Digest), and text editing and summarization tools (e.g. Paperpal, Quillbot, and Notion AI).

## Category 1: Interactive Response Generation

This category includes ChatGPT and similar systems like Google Bard. ChatGPT facilitates interactive communication by generating quick responses and incorporating a memory feature to recall previous inputs. While Google Bard shares similarities with ChatGPT, it is important to note that this study solely focused on ChatGPT, as only one system was needed for analysis due to how similar the systems function. These AI systems are versatile tools for

obtaining summaries on broad topics and performing various other tasks when prompted by the user.

# Category 2: Research Support and Analysis

Elicit, SciSpace Copilot, Writefull X, and Paper Digest all fall within this category, as these AI systems provide support for academic research tasks. Elicit provides relevant research articles and allows users to sort them based on criteria such as date or accessibility. Additionally, it generates citations, making it a valuable tool for sourcing trustworthy and well-cited research articles. SciSpace Copilot assists users in comprehending scientific articles through summarization. Writefull X offers features like title generation from abstracts, abstract generation from text, sentence paraphrasing, conversion of informal writing to academic styles, and identification of AI-generated text. Paper Digest focuses on summarizing articles, although its applicability is limited to articles with a DOI number.

## Category 3: Text Editing and Summarization Tools

Within this category are Paperpal, Quillbot, and Notion AI, which provide text editing and summarization functionalities for various types of content, including academic and non-academic texts. Paperpal suggests grammar edits based on a given text, facilitating text editing and refinement. Quillbot provides a wide range of capabilities including paraphrasing, grammar checking, plagiarism detection, co-writing, summarization, citation generation, and translation capabilities. Notion AI offers a wide range of functionalities, such as summarization, translation, grammar editing, text length adjustment, tone modification, language simplification, text explanation, and more. Moreover, Notion serves as a comprehensive tool with pre-designed templates for various types of content such as blog posts, emails, essays, and similar texts. It also

incorporates useful features like a user-friendly journal, task list, reading list, quick notes, and a memory function for generated text, similar to an agenda or journal.

# **Project Need**

The field of artificial intelligence (AI) has experienced rapid growth and holds significant potential for various applications in engineering. While previous research has focused on the ongoing development of new materials, little attention has been given to exploring the potential of AI in assisting engineers in this area. Additionally, there is a scarcity of research concerning the interaction between engineers and AI, particularly within the domain of materials engineering. Furthermore, the incorporation of AI in decision-making processes within this field remains largely unexplored.

The primary objective of this project was to harness the power of AI to enhance our understanding of the development of new materials, with a specific focus on a quaternary alloy system. By employing AI techniques, we aimed to research the development of new alloys that enhance desirable mechanical properties. Additionally, we sought to investigate how materials engineers interact with AI systems. To achieve this, we designed and conducted an extensive survey that included questions pertaining to the engineers' perception and experience with different AI systems. Furthermore, we developed a rubric to systematically evaluate how engineers perceive each AI system, providing valuable insights into their usability and effectiveness. Additionally, our research aimed to explore the decision-making process of materials engineers and their trust in AI technology. By gathering data on the engineers' decision-making practices and their perceptions of the reliability and trustworthiness of AI systems, we aimed to shed light on the potential barriers and opportunities for incorporating AI

within the materials engineering field. Furthermore, we conducted a case study on an engineer with limited experience in materials science, who utilized AI to write an academic paper on a quaternary alloy system (the CrCoNiFe alloy), documenting their firsthand experience and insights. The CrCoNiFe alloy is a variant of the famous CrCoNi system, which has been heavily studied due to its incredible combination of useful mechanical properties for many applications (Laplanche et al., 2017). Due to the success of the CrCoNi alloy and recent advances in modeling techniques, the addition of other elements has been studied in order to further improve material properties, but little success has been found so far. This Major Qualifying Project (MQP) in part aimed to help deliver a portion of an academic research paper on this topic for the Material Science PhD students at Worcester Polytechnic Institute (WPI) in Worcester, MA.

In summary, this project addressed a critical gap in the current research landscape by investigating the untapped potential of AI in materials engineers. By leveraging AI to gain deeper insights into the TWIP/ TRIP mechanisms, exploring the interaction between engineers and AI systems, and understanding the decision-making practices and perceptions of materials engineers, our research aims to contribute to the advancement of materials science and provide valuable guidance for future applications of AI in engineering contexts.

# Methods

### Approach

The goal of this study was to investigate how materials engineers can effectively leverage AI to facilitate the development of new materials. To achieve this objective, a comprehensive approach was adopted, starting with the creation of a rubric that served as the basis for the creation of a survey, which included open-ended, multiple-choice, and Likert-scale questions. To gain a thorough understanding of the diverse AI systems available on the market, a rubric was devised to assess each system according to specific criteria. The rubric underwent multiple iterations based on feedback from advisors, ensuring its effectiveness and relevance. Following this refinement process, both group members independently employed the rubric to evaluate eight AI systems: ChatGPT, Elicit, SciSpace Copilot, Writeful X, Paperpal, QuillBot, PaperDigest, and Notion. Following the initial evaluation of the AI systems, the rubric was incorporated into a survey that was subsequently distributed to materials engineers. The survey encompassed a range of question types, which explored participants' general perceptions and attitudes toward AI, their decision-making processes, and requested them to evaluate the same eight AI systems using the established rubric. To streamline the survey process, conditional formatting was employed, excluding materials engineers who had not previously utilized an AI system from scoring it using the rubric. In addition to evaluating AI systems, the survey aimed to gauge materials engineers' levels of trust in AI and their perceptions regarding its integration into the workforce for the advancement of new materials. Finally, a case study was conducted as an engineer used AI to write an academic paper on a quaternary alloy system, while documenting their firsthand experience and perceptions regarding the use of AI in the materials science field.

By encompassing these various aspects, the study sought to comprehensively explore the potential applications and implications of AI within the materials engineering domain.

# **Development of a Scoring Rubric**

In order to accurately assess the interaction between engineers and specific AI systems, a scoring rubric was developed to analyze each AI system based on specific criteria. The rubric aimed to facilitate research on each AI system and was subsequently incorporated into the survey (discussed later) to allow engineers to score the AI systems based on their experience.

The first draft of the rubric was created during the research phases of the project to enhance the understanding of each AI tool (refer to Table 1). The assessment of each AI system focused on the following criteria: ease of use, ability to generate citations, memory in past responses, accuracy of the generated responses, and speed of response generation. Each criterion was scored on a scale of three points, utilizing the following simple point scale:

- 0: Not present/not applicable.
- 1: Present and below average.
- 2: Present and average.
- 3: Present and above average.

*Table 1.* The first draft of the rubric.

	AI System 1	AI System 2	AI System 3
Ease of Use	/3	/3	/3
Citations	/3	/3	/3
Memory	/3	/3	/3
Accuracy	/3	/3	/3
Speed	/3	/3	/3
Total	/15	/15	/15

Although the initial draft was straightforward, a visually enhanced version of the rubric was subsequently developed. Additionally, in the second draft, the criterion of "citations" was removed as the text-editing AI systems were not designed to generate citations, and this criterion had a negative impact on the scores of many AI systems. Instead, it was replaced with the criterion of "trustworthiness" to allow participants to subjectively evaluate how much they trusted each AI system, regardless of whether citations were provided. Furthermore, an additional row was added, labeled "category," to group the AI systems based on their functions for easier score comparison of similar AI systems. Employing the same criteria as presented in Table 1, with the exchange of the "citations" criterion for "trustworthiness" and the addition of a categorization row, a hypothetical example of the color-coded second draft rubric is illustrated in Table 2. The following color codes were used for the criteria scores:

- 0: Not present/not applicable.
- 1: Present and below average.
- 2: Present and average.
- 3: Present and above average.

Similarly, the color codes for the total scores were as follows:

- 0 /15 4.9/15.
- 5/15 9.9/15.
- 10/15 15/15.

**Table 2.** A hypothetical example of the second draft of the rubric.

Category	Category 1	Category 2	Category 3
AI System	AI System 1	AI System 2	AI System 3
Ease of Use	3/3	2/3	1/3
Trustworthiness	2/3	3/3	1/3
Memory	3/3	0/3	0/3
Accuracy	2/3	2/3	0/3
Speed	2/3	2/3	2/3
Total	12/15	9/15	4/15

Note: The values in Table 2 are hypothetical and are provided as an example of the color-coded rubric.

# Survey to Deconstruct Materials Engineers' Perceptions of AI

In order to gain a comprehensive understanding of the interaction between materials engineers and specific AI systems, as well as engineers' perceptions of AI and their decision-making processes, a Qualtrics survey was developed. The survey aimed to incorporate a variety of question types to capture different aspects of the materials engineers' experiences and perspectives (see Appendix A). The survey included open-ended, multiple-choice, and Likert-scale questions. Open-ended questions enabled respondents to provide detailed feedback in their own words, while multiple-choice questions provided a structured and standardized

approach for data collection. The Likert-scale questions allowed participants to indicate their feelings and attitudes on a standardized scale, which provided a consistent measure of their opinions. By incorporating three different question types, the survey aimed to gather a comprehensive range of data and perspectives from the engineers, allowing for a deeper exploration of the research objectives.

As previously mentioned, the rubric developed to assess AI systems was incorporated into the survey, enabling engineers to express their sentiments towards specific AI systems. The AI systems assessed in the survey included ChatGPT, Elicit, SciSpace Copilot, Writeful X, Paperpal, QuillBot, PaperDigest, and Notion. Participants were asked to score each AI system using the same criteria outlined in Table 2 (the second draft of the rubric). However, it is important to note that the rubric within the survey was not color-coded, as Qualtrics does not provide this functionality. The scoring results from the participants were later color-coded according to the score criteria during the analysis phase and are further discussed in the subsequent sections.

Additionally, to enhance the survey's efficiency and tailor the questionnaire to individual respondents, a conditional formatting approach was implemented. The survey was designed to present questions based on the participants' specific answers, ensuring that they only received relevant inquiries. For instance, if respondents indicated in prior question(s) that they had never heard of or used ChatGPT, they were not presented with additional questions concerning that particular AI system. This conditional formatting approach minimized participant burden by focusing the survey on areas directly relevant to their experiences and knowledge. The inclusion of specific follow-up questions for each AI system allowed for a comprehensive assessment of engineers' perceptions and experiences with the different AI systems. The additional questions

for each AI system can be seen in Appendix A. By customizing the survey based on respondents' previous answers, we ensured a streamlined and targeted data collection process. This approach allowed for more precise insights into engineers' interactions and opinions regarding the AI systems under investigation. The survey was designed to be anonymous, and participants were required to provide informed consent by agreeing to it. Furthermore, all questions were optional and could be skipped.

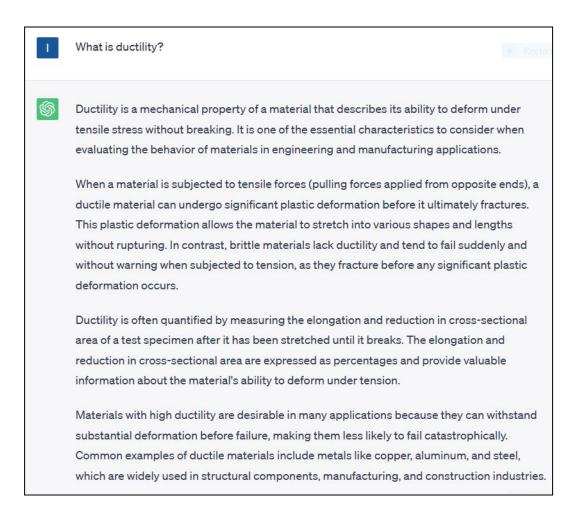
## Case Study: Using AI to Accelerate Materials Discovery

A case study was conducted to analyze the effectiveness of AI use in crafting an academic research paper in the area of material science. A WPI material science PhD student presented to the MQP team members their current research area and a topic for a research paper. This presentation introduced the team to research in the material science field, background on material science and gave the team perspective on the end goal of the project, an introduction and literature review of an academic paper on a material science topic of the team's choosing. An engineer on the MQP team with limited material science background was tasked with writing, using AI tools on a limited schedule, the introduction and literature review of a paper on the CrCoNiFe alloy. Usually a person writing a paper of this kind would have been trained in material science at least with an undergrad or graduate degree. The task of the research project was to find if, with the help of AI, an engineer with limited material science background could quickly write a similar paper, ideally in two days. Information given in the PhD student's presentation, while helpful for understanding the current state of material science research and his own research, did not provide much context on the specific alloy of discussion, the CrCoNiFe alloy. Some information from the presentation was used as context for the introduction section of the paper, but more information was necessary for the engineer to write a successful introduction and literature review.

Due to the popularity of the ChatGPT AI tool, the platform was used initially for research and general questions for the engineer to gain a more thorough understanding of the subject matter. Information from ChatGPT heavily influenced the introduction section of the academic paper. ChatGPT was very convenient for quickly getting concise answers to questions in the research process and was decently accurate in its responses, which is known because the material engineering PhD student who reviewed the introduction section later upheld that it was accurate. Without the help of a subject matter expert, the information from ChatGPT would have had to be confirmed through research as its claims are not guaranteed to be accurate and are not substantiated with any sources as shown in Figures 2 and 3 (see Appendix B for all AI questions and answers).

ChatGPT may produce inaccurate information about people, places, or facts. ChatGPT August 3 Version

**Figure 2.** ChatGPT includes a warning below the message box that it may provide inaccurate information.

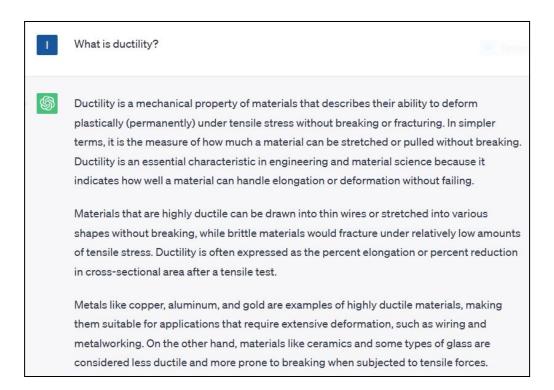


*Figure 3.* ChatGPT answers are given with no resources to back up their claims.

While the information ChatGPT provides is not backed up with sources, using ChatGPT was much quicker than traditional research using a search engine. This made the AI tool useful for basic research questions and becoming familiar with the terminology of a research area that was previously unknown to the engineer, but the lack of source information hindered the literature review process. Another drawback to the tool was that ChatGPT is only able to complete 25 searches in 4 hours, so it is not able to accommodate every simple question a person who is new to a subject may have in a timely manner. Although this could be an issue for some researchers, this feature did not impact the engineer's research too heavily since the answers from ChatGPT can be very detailed and sometimes lengthy, so they were found to be enough to

sustain research practices without going over the search limit. While ChatGPT responses can be detailed, they did not always contain the information needed by the engineer to accurately summarize a paper. If this occurred, the engineer could go back to the text and read it themselves, ask a more direct question to ChatGPT, or regenerate the response.

One feature of ChatGPT that proved to be helpful for the research and writing process was the regeneration tool. When there was a lengthy or difficult answer, then the regeneration tool could give a similar response in different language and perhaps some new information that helped to digest concepts more quickly and accelerate the research and learning process. For example, when asked to regenerate the prompt "What is ductility?" (see Figure 3) ChatGPT was able to provide a similar answer with the same general information, but with some new information, such as plastic deformation meaning permanent deformation and wiring and metalworking being suitable applications for highly ductile materials (Figure 4).



**Figure 4.** The regeneration feature provides a similar answer to a prompt with new or different information.

Another drawback to ChatGPT is that its knowledge is currently cutoff in September 2021, so all of the newest areas of research are not included in the responses, making it only useful for background information and quick answers to more simple questions. When asked to provide information about current research, ChatGPT can give basic information, but ultimately refers the user to up to date information given through other sources (Figure 5).

Remember that the field of materials science is continuously evolving, and researchers around the world are actively contributing to new advancements in HEAs and the CrCoNiFe system. To get the latest and most accurate information on recent research, I recommend checking scientific journals, conference proceedings, and academic databases for publications from 2022 and 2023.

*Figure 5.* ChatGPT recommends other research avenues for up to date information.

Given prompts, ChatGPT was useful to find information quickly, but it proved difficult for an engineer without an educational background on materials science to come up with important concepts to include in a paper. In order to find research areas and streamline the writing process, the Notion AI tool was used to outline important sections to be included in the Introduction of a paper of this type as well as prompts to ask ChatGPT to elaborate on. When asked to Outline the CrCoNiFe System, Notion was able to come up with a list of information to include, such as the microstructure, mechanical properties, and applications of the system.

# **Cr-Co-Ni-Fe System Outline**

The Cr-Co-Ni-Fe system is a group of alloys that consist of chromium (Cr), cobalt (Co), nickel (Ni), and iron (Fe). These alloys are known for their excellent mechanical and corrosion properties, making them ideal for use in various applications. In this outline, we will discuss the important aspects of the Cr-Co-Ni-Fe alloy system.

#### Introduction to Cr-Co-Ni-Fe system

The Cr-Co-Ni-Fe system is a popular alloy system used in various engineering applications due to its excellent properties. The system has a wide range of compositions that can be tailored to suit various applications.

#### Composition and properties of Cr-Co-Ni-Fe alloys

The composition of Cr-Co-Ni-Fe alloys can vary widely, and the properties of the alloy are dependent on the composition. The addition of different elements can change the mechanical, corrosion, and physical properties of the alloy. The properties of these alloys make them ideal for use in industries such as aerospace, marine, and chemical.

#### Microstructure of Cr-Co-Ni-Fe alloys

The microstructure of Cr-Co-Ni-Fe alloys plays a significant role in determining the properties of the alloys. The microstructure can be controlled through various processing techniques such as heat treatment and casting. The microstructure can be modified to achieve different properties such as high strength or high corrosion resistance.

### Mechanical properties of Cr-Co-Ni-Fe alloys

The mechanical properties of Cr-Co-Ni-Fe alloys are excellent, and they exhibit high strength, toughness, and ductility. These alloys have a good balance of strength and ductility, making them ideal for use in structural applications.

#### Corrosion resistance of Cr-Co-Ni-Fe alloys

The corrosion resistance of Cr-Co-Ni-Fe alloys is excellent, and they are resistant to various types of corrosion such as pitting, crevice, and stress corrosion cracking. The corrosion resistance of these alloys makes them ideal for use in harsh environments such as marine and chemical industries.

#### Applications of Cr-Co-Ni-Fe alloys

Cr-Co-Ni-Fe alloys are used in various applications such as aerospace, marine, chemical, and nuclear industries. These alloys are used in the manufacture of gas turbines, aircraft engines, chemical processing equipment, and nuclear reactors.

In conclusion, the Cr-Co-Ni-Fe alloy system is a highly versatile and useful group of alloys that have excellent properties. The properties of these alloys make them ideal for use in various applications, and they are widely used in industries such as aerospace, marine, and chemical.

**Figure 6.** Notion is helpful for outlining important concepts and research areas.

Background information on materials science from ChatGPT and Notion was useful in the preparation of the introduction, but when ChatGPT was tested to find academic papers it created imitation sources that appeared to be real, but did not exist. Without up-to date information or academic sources, ChatGPT could not be used heavily for the literature review section, so other AI tools were tested.

In order to create a literature review of the alloy, a number of academic sources had to be found, read, and summarized. This can be a lengthy process since it requires the engineer to absorb a lot of information from various researchers who present their findings in different ways. The AI platform SciSpace Copilot was tested to be used in the literature review process, since it is marketed to help researchers digest the many academic papers in its database as well as academic papers uploaded to the tool quickly and efficiently, but it was found to give incorrect information when summarizing. When using a suggested function of the AI tool, to summarize an abstract in 2 sentences, the tool gave a summary that was incorrect and irrelevant to the abstract of the paper it was asked to summarize.

Qillbot was not used in the case study preparation since its primary use was to paraphrase and that function was not as necessary to the writing process as summarization. PaperDigest also proved to be unhelpful during the case study since its site was no longer maintained because a new version is projected to release soon. Elicit was found to be more helpful in the literature review process as it helped to summarize findings, check the relevancy of papers, and helps to find papers quickly. It was used as an upgraded search engine to accelerate the finding of academic papers by giving a short abstract summary as well as evaluating the trustworthiness of the paper. While it worked quickly and was able to filter out relevant papers, not all of its features could be used for every article as some articles did not provide information on the trustworthiness of the paper. Elicit was very helpful at the beginning of the literature review process and was able to locate academic papers that were relevant to the prompts it was given,

but other than the short abstract summary given by Elicit, it could not summarize the details of the academic papers.

ChatGPT was employed as a tool for summarization of academic papers relevant for the literature review of the CrCoNiFe alloy. At times ChatGPT was successful in summarizing academic papers and saving the engineer time deciphering long texts, but other times it was unable to do so. Sometimes when given a URL to an academic paper, ChatGPT was able to come up with a summary of the paper and its findings, but other times it would give an error message, as shown in Figure 7.



I'm sorry, but as a text-based AI, I cannot directly view or access files, images, or documents you may have. However, if you can provide the title, abstract, or key points from the academic paper, I'd be happy to help summarize or explain it.

Figure 7. Error message from ChatGPT when asked to summarize an academic paper.

Pasting text directly into the "Send a message" box in ChatGPT generally worked to summarize, as long as the pasted text was not too lengthy. Some academic papers were too lengthy for ChatGPT to summarize so the engineer had to paste only sections or the abstract for the AI tool to summarize. The summaries saved time that would have been spent reading most or all of an academic paper to understand the theory behind the project and its outcomes. Instead, the summaries could be used to aid in writing about the academic papers in the literature review of the paper.

After creating a draft of the introduction and literature review Paperpal was helpful in editing and helping with wording to make the paper sound more scholarly. This was especially helpful for a writer with little experience writing academic papers, so this AI helped cut down on editing time substantially. Writefull X was also tested as part of the survey for editing, but

ultimately was not used since it was redundant to Paperpal and Paperpal was more useful for solely editing purposes. If an abstract were expected as part of the delivery then Writeful X would have been used due to its abstract and title generator.

After a first draft using AI tools, the introduction and literature review were given to a material science PhD student for review. The introduction and literature needed more citations to back up claims made and other minimal edits. Since the information used from ChatGPT to create the introduction did not have sources to back up its claims, sources had to be found to prove the statements made were true. The number of sources Elicit was able to find specifically on the topic of the CrCoNiFe was not substantial enough for the introduction and literature review, so traditional researching methods had to be used to add more academic sources to back up the claims made in the introduction and literature review. Google Bard was also sampled towards the end of the project to see its effectiveness in researching, but was found to be similar to ChatGPT as it only was able to provide sources that do not exist. When tasked with summarizing, Bard was found to be less detailed and therefore not as helpful as ChatGPT. After the first draft one transition paragraph was also added after the introduction to more explicitly convey the need of the paper. The final introduction and literature review produced from the case study, along with all references used can be seen in Appendix C.

### **Analysis**

### Analysis: Initial Evaluation of AI Systems

For the initial evaluation of AI systems, both group members utilized the developed rubric to score each of the eight AI systems: ChatGPT, Elicit, SciSpace Copilot, Writeful X, Paperpal, QuillBot, PaperDigest, and Notion. The rubric encompassed several criteria, including

ease of use, trustworthiness, memory for past responses, accuracy in generating responses, and response generation speed. Each criterion was scored on a scale of 0 to 3 points, resulting in a cumulative score ranging from 0 to 15. The individual scores from both group members were averaged to derive the final scores for each AI system. This scoring process allowed for a comprehensive assessment of the AI systems' performance across multiple dimensions, providing valuable insights into their strengths and weaknesses. The average scores served as quantitative indicators of the system's overall effectiveness, adding in subsequent analysis and comparison of their capabilities for materials engineers.

### Analysis: Materials Engineers' Evaluation of AI Systems

After the survey was developed, it was distributed to a diverse group consisting of undergraduate students, graduate students, and faculty members specializing in materials engineering. The purpose of this survey was to gather valuable insights into the perceptions and decision-making processes of professionals within the field. A total of 10 responses were received, which provided a basis for the subsequent analysis. The collected responses were carefully examined to gain a comprehensive understanding of various aspects related to the usage of AI systems in materials engineers. Specifically, the analysis focused on evaluating the perceptions and opinions of the participants regarding eight specific AI systems. By examining their responses, we sought to uncover insights into how material engineers make decisions and their overall perception of AI's potential in the development of new materials. The analysis of the received responses involved a systematic examination of the data, which encompasses both qualitative and quantitative approaches. Through this process, we aimed to identify common patterns, trends, and themes emerging from the participant's feedback, while also comparing the

results to the initial analysis of the eight AI systems. By leveraging the diversity of perspectives within the participant group, we strived to capture a comprehensive view of the subject matter.

### Analysis: Materials Engineer Case Study

A case study was conducted to investigate the application of AI systems in the domain of materials science. The study focused on a materials engineer who utilized AI systems to write an academic paper on a quaternary alloy system. Throughout the case study, the engineer documented their firsthand experience, thoughts, and perceptions of employing AI in the materials science domain, providing valuable insights into the practical implementation of AI technologies. The engineer's experience with various AI systems was thoroughly examined, enabling a comprehensive analysis of the advantages, challenges, and limitations associated with AI adoption in the field. By utilizing a range of AI systems specifically designed for academic writing, the engineer was able to evaluate their effectiveness, efficiency, and overall impact on the research process. The material engineer's survey response was also examined as it provided a structured way for the engineer to document their experience and thoughts while using AI. Through the combination of the engineer's firsthand experience and their survey response, this case study offers an examination of the utilization of AI systems in academic research. By documenting the engineer's personal insights and survey results, we aim to shed light on the current state of AI implementation in material science and identify areas for improvement or further exploration.

### **Results**

### **Initial Evaluation of AI Systems**

In order to gain a better understanding of the AI systems before asking engineers about their perspectives, a comprehensive assessment was conducted by the group. The rubric presented in Figure 2 was utilized to evaluate a total of eight AI systems: ChatGPT, Elicit, SciSpace Copilot, Writefull X, Paperpal, QuillBot, Paper Digest, and Notion. Both group members independently evaluated the AI systems using the rubric and took note of their experience. The individual and average scores for each AI system, along with their combined notes are described below. The AI systems were grouped by function using the same categories that were employed in the *AI Systems* section, which can be seen in Tables 3-5.

As for ChatGPT, this system serves as an interactive tool capable of generating quick responses. Notably, it possesses a memory feature that enables it to recall previous inputs. In addition, it is a convenient tool to gain a summary of a broad topic and responses can be regenerated which creates re-worded responses with some additional information. Despite these advantages, it is important to highlight that ChatGPT lacks citations for its responses, which presents a challenge for researchers seeking to utilize it in academic papers. Additionally, this absence of citations may lead engineers to question the reliability and trustworthiness of the generated responses. Furthermore, the system imposes a limit of twenty-five searches within a four-hour timeframe, which may prove restrictive for some users. It is worth noting that, on occasion, the responses produced by ChatGPT are not entirely accurate, lack visual aids such as images or diagrams, and exhibit a tendency to employ repetitive adjectives and vocabulary.

Group member one's rubric can be seen in Table 3, while group member two's rubric can be seen

in Table 4. Both group members gave ChatGPT a score of 12 out of 15, giving it an average score of 12 out of 15, positioning it within the high-scoring category, as seen in Table 5.

As for Elicit, this particular AI system excels at swiftly providing relevant research articles that can be sorted based on various criteria such as date or accessibility. When a specific article is selected, Elicit furnishes the user with the abstract, a summary, measured outcomes, participant information, and reasons to trust the article. In contrast to ChatGPT, Elicit generates citations for its responses, making it an excellent tool for sourcing trustworthy and well-cited research articles. However, it is important to note that not all features of Elicit can be utilized with every article. Group member one gave Elicit a score of 10 out of 15, while group member two gave it a score of 9 out of 15. The average total score of 9.5 out of 15, places Elicit in the top of the middle-scoring category of AI systems, as presented in Table 5.

SciSpace Copilot is an AI system that helps users to comprehend scientific articles through summarization. It has a large database of articles and provides links to related papers, however, despite its extensive data repository, many of the responses generated by SciSpace Copilot were found to be inaccurate. For instance, when asked to summarize an abstract, the systems referred to wind turbines, which were never mentioned in the original paper.

Additionally, SciSpace Copilot is comparatively slower in generating responses and only provides a summary, omitting the full-text of the article. Consequently, based on this evaluation, group member one gave SciSpace Copilot a score of 4 out of 15, while group member two gave it a 3 out of 15. The average total score of 3.5 out of 15, places SciSpace Copilot in the low-scoring category, as indicated in Table 5.

Writefull X is an AI system that is very each to use and includes a variety of specific functions, such as generating titles from abstracts, generating abstracts from text, paraphrasing

complex sentences, converting informal writing to academic style, and identifying text generated by AI systems like ChatGPT or a similar models. Writefull X demonstrates high accuracy in its responses and provides fast outputs, however, a notable drawback is its lack of memory for past inputs. Each input is treated as a separate task, making it challenging to switch between functions. For example, if the user wants to generate a title after entering text for an abstract, a separate input must be provided on a different page. Additionally, Writefull X has a limitation in the amount of text it can process, usually limited to a few sentences. Another drawback is the system's inability to generate citations. In our evaluation, both group members rated Writefull X with a score of 9 out of 15, which places Writefull X in the middle-scoring category, as shown in Table 5.

Paperpal is an AI system that focuses on suggesting grammar edits based on a given text. Its notable advantage is the seamless integration with Word, making it easily accessible for users. However, Paperpal lacks a wide range of functions and tends to be slower in generating responses compared to other AI systems. One concern raised during the evaluation is the contradictory grammar suggestions provided by Paperpal in comparison to other AI systems. Group member one gave Paperpal a score of 7 out of 15, while group member two rated it slightly higher with a score of 9 out of 15. The average score of 8 out of 15 places Paperpal in the middle-scoring category, as shown in Table 5.

Quillbot stands out among the AI systems evaluated due to its extensive set of features. It offers paraphrasing, grammar checking, plagiarism detection, co-writing, summarization, citation generation, and translation capabilities. The system is user-friendly, accessible across different web browsers, and provides generous text/character limits in the free version. However, similar to Writefull X, Quillbot does not have a memory for past inputs. Both group members found

Quillbot easy to use and appreciated the availability of citation generation. Both group members scored Quillbot with a 9 out of 15, which places Quillbot in the top of the middle-scoring category, as seen in Table 5.

Paper Digest focuses on summarizing articles; however, it only works with articles that have a DOI number, limiting its applicability. Furthermore, the summaries generated by Paper Digest are overly brief, comprising only three general sentences to summarize extensive papers. Both group members expressed dissatisfaction with the user experience and found the system difficult to use. Both group members gave Paper Digest a score of 4 out of 15, which places Paper Digest in the low-scoring category, as shown in Table 5.

Lastly, Notion AI offers a wide range of functionalities, including summarization, translation, grammar editing, text length adjustment, tone modification, language simplification, text explanation, and more. Moreover, Notion serves as a comprehensive tool with pre-designed templates for various types of content such as blog posts, emails, essays, and similar texts. It also incorporates useful features like a user-friendly journal, task list, reading list, quick notes, and a memory function for generated text, similar to an agenda or journal. However, one drawback is that, unlike other AI systems like ChatGPT, Notion requires selecting an option from a limited set of choices when given a task. This slightly slows down the process of engaging with the AI, although the response generation itself is highly efficient. Additionally, Notion is only capable of performing tasks within its available options and cannot handle requests beyond that scope.

Group member one gave Notion a score of 12 out of 15, while group member two gave it a score of 13 out of 15. The resulting total average score of 12.5 out of 15, places Notion in the high-scoring category, as indicated in Table 5.

In analyzing the scores and evaluations provided by the two group members, it is evident that both shared similar perspectives on the performance of the AI systems. Both group members were in agreement for the scores of four out of the eight AI systems, indicating a consensus in their evaluations. However, slight discrepancies were observed in the scores of the other four AI systems, where the group members differed by 1 point for three of the AI systems, and the final AI system showed a 2-point difference. These variations in scores between the group members could be attributed to individual preferences, perspectives, or experiences with the AI systems. It is important to consider these differences as they provide valuable insights into the subjective nature of evaluating AI systems. By acknowledging and discussing these discrepancies, a more comprehensive understanding of the strengths and weaknesses of each AI system can be obtained. Overall, despite the variation in scores, the evaluations conducted by both group members contribute to a well-rounded assessment of the AI systems, highlighting their distinct features and limitations.

**Table 3.** Group member one's initial rubric scores for AI systems.

Category	Interactive Response Generation	Research Support and Analysis				Text Editing and Summarization Tools		
AI System	ChatGPT	Elicit	SciSpace Copilot	Writefull X	Paper Digest	QuillBot	Paperpal	Notion
Ease of Use	3/3	2/3	2/3	1/3	1/3	2/3	3/3	3/3
Trustworthiness	2/3	3/3	1/3	2/3	1/3	3/3	1/3	2/3
Memory	3/3	0/3	0/3	0/3	0/3	0/3	0/3	3/3
Accuracy	2/3	3/3	0/3	3/3	0/3	2/3	2/3	2/3
Speed	2/3	2/3	1/3	3/3	2/3	2/3	1/3	2/3
Total	12/15	10/15	4/15	9/15	4/15	9/15	7/15	12/15

Table 4. Group member two's initial rubric scores for AI systems.

Category	Interactive Response Generation	Research Support and Analysis			Text Editing and Summarization Tools			
AI System	ChatGPT	Elicit	SciSpace Copilot	Writefull X	Paper Digest	QuillBot	Paperpal	Notion
Ease of Use	3/3	2/3	2/3	2/3	1/3	2/3	3/3	3/3
Trustworthiness	2/3	2/3	0/3	2/3	1/3	3/3	2/3	2/3
Memory	3/3	0/3	0/3	0/3	0/3	0/3	0/3	3/3
Accuracy	2/3	3/3	0/3	2/3	1/3	2/3	2/3	2/3
Speed	2/3	2/3	1/3	3/3	1/3	2/3	2/3	3/3
Total	12/15	9/15	3/15	9/15	4/15	9/15	9/15	13/15

*Table 5.* Average rubric scores for AI systems from both group members.

Category	Interactive Response Generation	Research Support and Analysis			Text Editing and Summarization Tools			
AI System	ChatGPT	Elicit	SciSpace Copilot	Writefull X	Paper Digest	QuillBot	Paperpal	Notion
Group Member One	12/15	10/15	4/15	9/15	4/15	9/15	7/15	12/15
Group Member Two	12/15	9/15	3/15	9/15	4/15	9/15	9/15	13/15
Average	12/15	9.5/15	3.5/15	9/15	4/15	9/15	8/15	12.5/15

### Materials Engineers' Perceptions and Evaluations of AI

### Perceptions of AI

To assess materials engineers' opinions about AI, a Qualtrics survey was designed and distributed to a diverse group of materials engineers, following IRB approval. The survey

comprised a total of sixty-eight questions, including open-ended, multiple-choice, and Likert-scale questions (Appendix A). Open-ended questions enabled respondents to provide detailed feedback in their own words, while multiple-choice questions provided a structured and standardized approach for data collection. The Likert-scale questions allowed participants to indicate their feelings and attitudes on a standardized scale, which provided a consistent measure of their opinions. By incorporating three different question types, the survey was able to capture a range of data and perspectives from the participants.

The survey had an average completion time of 11.63 minutes, and a total of n=10 materials engineers participated. The participants encompassed undergraduate and graduate student materials engineers, as well as professors in materials engineering. All participants indicated their field of study, confirming their affiliation with materials science, with specific areas such as "solid-state electrolytes in lithium-ion batteries" and "molten salt by molecular dynamics" mentioned. This ensured that the responses collected were from individuals working in the materials science field, validating the data. Furthermore, participants were asked to self-identify as engineers, with 3 participants strongly affirming their engineer status, 6 participants leaning towards considering themselves engineers, and 1 participant being uncertain (Figure 8).

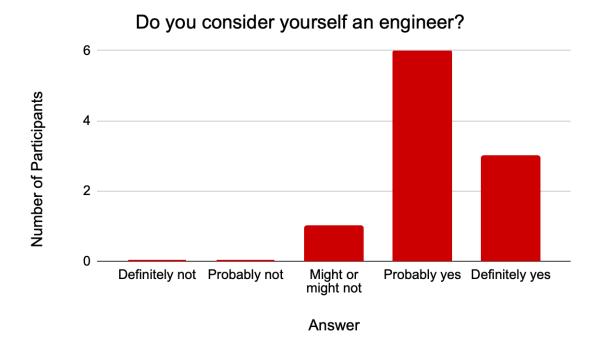


Figure 8. Results from the survey to the question "Do you consider yourself an engineer?"

At the beginning of the survey, participants were asked to share their general perceptions of AI and its utility for engineers. All participants indicated that they believe that "it will be very powerful someday in the future" and has "tremendous potential." When rating their feelings about using AI on a scale of 1 to 5, with 1 representing "very hesitant" and 5 representing "very eager," the average rating fell between 2 and 5, with an overall average of 3.80. Specifically, 2 participants expressed "somewhat hesitant," 6 participants indicated "somewhat eager," and 2 participants expressed "very eager" (Figure 9). When asked to explain their choice, many who indicated eagerness said "I believe it's the trend for the future," and those who indicated hesitancy said, "The training of an AI model will need lots of data and [it will be] time consuming."

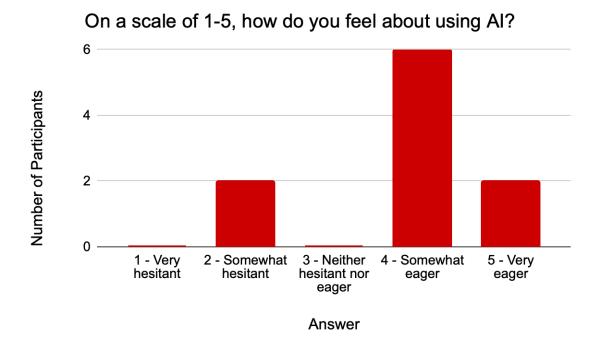
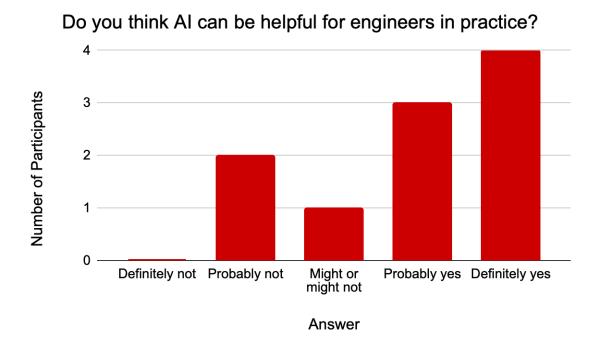


Figure 9. Results from the survey to the question "On a scale of 1-5, how do you feel about using AI?"

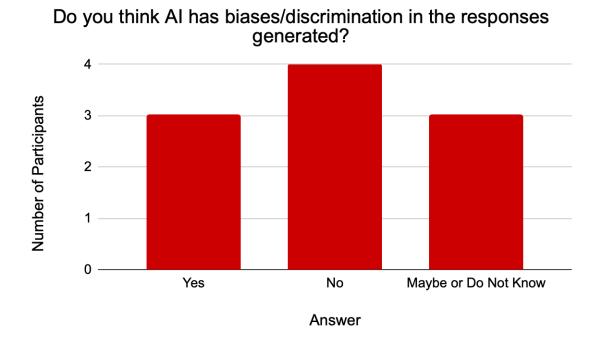
Participants were then asked to evaluate the usefulness of AI for engineers in practice. As seen in Figure 10, responses varied on a 5-point scale, with 1 representing "definitely not" and 5 representing "definitely yes." The average score was 3.90, indicating a positive outlook overall. Specifically, 2 participants expressed "probably not," 1 participant indicated "might or might not," 3 participants indicated "probably yes," and 4 participants expressed "definitely yes." There are several reasons to explain this discrepancy, including the participants' varying levels of familiarity with using AI, the applicability of AI in their specific materials science domain, and their individual attitudes toward adopting new technologies within their field.



**Figure 10.** Results from the survey to the question "Do you think AI can be helpful for engineers in practice?"

The survey also aimed to explore participants' perceptions of AI biases and discrimination. When asked if AI systems has biases or discrimination in their responses, 3 participants answered "yes," 4 participants answered "no," and 3 participants answered "maybe" or "do not know" (Figure 11). Among the two participants who affirmed experiencing bias or discrimination in AI-generated responses, one cited "ChatGPT" as the source, while the other attributed it to "limited input." There are several reasons to explain this discrepancy, including the participants' varying levels of exposure to AI, their understanding of bias, the specific AI systems they typically use, and their personal experiences with AI, which may have influenced their perceptions regarding biases or discrimination in AI-generated responses. Participants were further asked to rate their trust in AI on a 5-point scale, with 1 indicating "none at all" and 5 indicating "a great deal." As seen in Figure 12, the responses ranged from 2 to 4, with an average

of 3.10. Specifically, 2 participants expressed "a little" trust, 5 participants expressed "a moderate amount" of trust, and 3 participants expressed "a lot" of trust.



**Figure 11.** Results from the survey to the question "Do you think AI has biases/discrimination in the responses generated?"

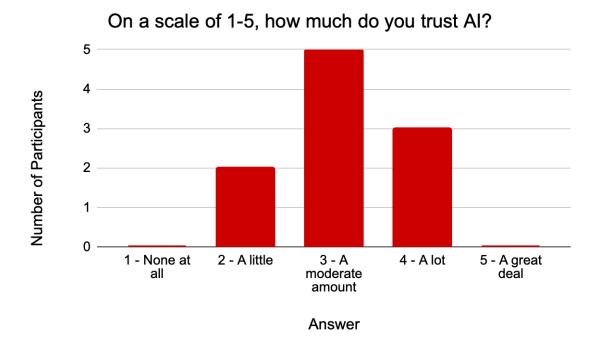
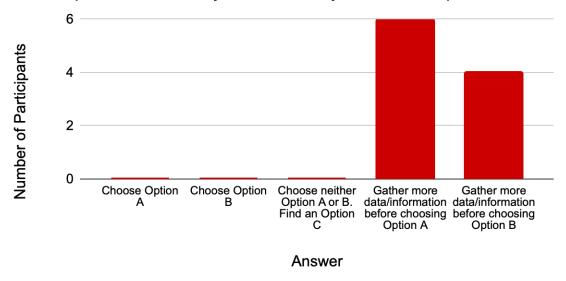


Figure 12. Results from the survey to the question "On a scale of 1-5, how much do you trust AI?"

Participants were presented with a hypothetical scenario: "What would you do in this scenario: you are an experienced engineer working to solve a problem. Your "gut-feeling" is telling you to choose Option A, but when you ask AI it says to choose Option B." They were given several response options: "choose Option A," "choose Option B," "choose neither Option A or B. Find an Option C," "gather more data/information before choosing Option A," and "gather more data/information before choosing Option B." As seen in Figure 13, the results showed that all participants opted to "gather more data/information before choosing Option A" or "gather more data/information before choosing Option B." Ultimately, 6 participants chose Option A, while 4 participants chose Option B.

What would you do in this scenario: you are an experienced engineer working to solve a problem. Your "gut-feeling" is telling you to choose Option A, but when you ask AI it says to choose Option B.



**Figure 13.** Results from the survey to the hypothetical scenario: "What would you do in this scenario: you are an experienced engineer working to solve a problem. Your 'gut-feeling' is telling you to choose Option A, but when you ask AI it says to choose Option B."

Following this, participants were asked if they had any concerns about using AI as an engineer, and 3 participants responded with "N/A," while the remaining 7 participants expressed their concerns. Their concerns included "data fabrication in training models" and "the [lack of] solid support of the database." Additionally, participants were questioned about their belief in whether AI protects user data. Responses were recorded on a 5-point scale, ranging from "definitely not" (1) to "definitely yes" (5). The average response fell at 2.56, with 1 participant choosing "definitely not," 3 participants selecting "probably not," 4 participants stating "might or might not," and one participant responding "probably yes." The final participant expressed uncertainty by stating "I do not know" (Figure 14).

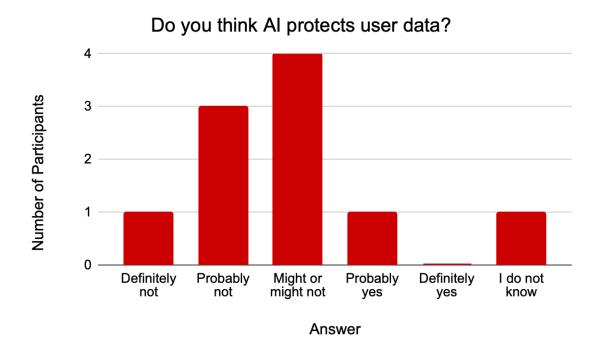
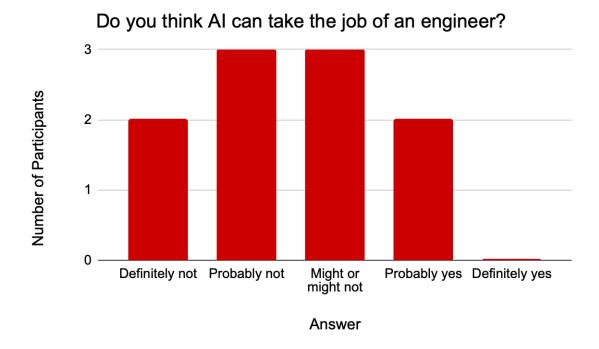


Figure 14. Results from the survey to the question "Do you think AI protects user data?"

Participants were also asked about their opinions on whether AI could replace the job of an engineer. Using the same 5-point scale, responses ranged from 1 to 4, with an average score of 2.50. As seen in Figure 15, 2 participants firmly believed that AI could not replace an engineer's job ("definitely not"), 3 participants were inclined towards "probably not," 3 participants expressed uncertainty by choosing "might or might not," and two participants believed that AI could "probably yes" replace the job.

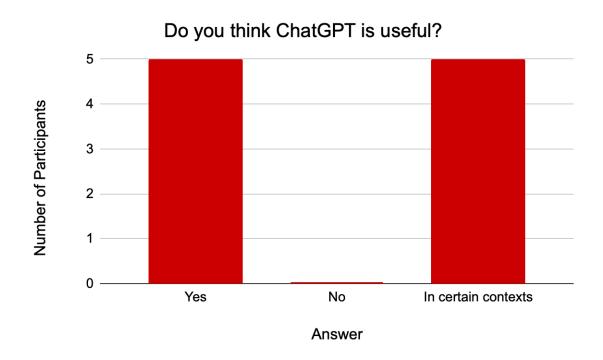


**Figure 15.** Results from the survey to the question "Do you think AI can take the job of an engineer?"

### AI Systems Evaluations

After assessing the general perceptions of materials engineers regarding AI, participants were asked about specific AI systems: ChatGPT, Elicit, SciSpace Copilot, Writeful X, Paperpal, QuillBot, PaperDigest, and Notion. To optimize the survey's efficiency and tailor it to individual respondents, a conditional formatting approach was employed. If participants indicated in previous questions that they were unfamiliar with or had not used a specific AI system, they were not presented with further questions about that particular system. This approach aimed to minimize participant burden by focusing on areas relevant to their experiences and knowledge. Participants who had used a specific AI system were asked to fill out the same rubric used in the initial evaluation of the AI systems.

The evaluation started with ChatGPT. All ten participants confirmed that they had both heard of and used ChatGPT before. Since all participants had used it, they were then asked about their perception of the AI system. First, participants were asked if they found ChatGPT useful, resulting in a split response, with five participants answering "yes" and five participants responding with "in certain contexts." No participants indicated that they believed ChatGPT was not useful (Figure 16).



*Figure 16.* Results from the survey to the question "Do you think ChatGPT is useful?"

Participants were then asked to complete a rubric evaluating ChatGPT based on the following criteria: ease of use, trustworthiness, memory of past responses, accuracy of generated responses, and speed of response generation. Each criterion was scored on a scale of three points, using the following simple point scale:

- 0: Not present/not applicable.
- 1: Present and below average.

- 2: Present and average.
- 3: Present and above average.

The average scores for each criterion for ChatGPT are as follows: ease of use (M = 2.6), trustworthiness (M = 1.8), memory of past responses (M = 2.2), accuracy of generated responses (M = 1.7), and speed of response generation (M = 2.6) (Table 6). This resulted in a total average score of 10.9, which is 1.1 lower than the initial average score of 12 points obtained in our evaluation of ChatGPT.

**Table 6.** Average survey scores for ChatGPT from 10 participants.

	ChatGPT - AVERAGE
Ease of Use	2.6/3
Trustworthiness	1.8/3
Memory	2.2/3
Accuracy	1.7/3
Speed	2.6/3
Total	10.9/15

Participants were then asked to share their general impressions of ChatGPT. Most participants described it as "very powerful and helpful," while others mentioned that it was "efficient but needs improvement in terms of reliability." When asked about likes and dislikes, participants commented that "sometimes the information is not accurate" and "data resources are limited."

Subsequently, participants were asked about several other AI systems. Regarding Elicit, none of the participants had heard or used it, so they were not asked to provide their feelings or complete the rubric. The same response was received for Writefull X, Paperpal, and Paper Digest. In the case of SciScace Copilot, 2 out of the 10 participants had heard of it, but neither

had used it. The same result was found for Notion AI. Regarding Quillbot, 2 of the 10 participants had heard of the AI system, but only 1 had used it. The participant who had used Quillbot found it useful, and their rubric scores can be seen below in Table 7:

**Table 7.** Survey scores for Quillbot from 1 participant.

	Quillbot
Ease of Use	3/3
Trustworthiness	2/3
Memory	0/3
Accuracy	1/3
Speed	2/3
Total	8/15

There is a 1-point difference in the total score of Quillbot compared to the average score of 9 points from our initial evaluation of Quillbot. When asked about their general feelings regarding Quillbot, one participant described it as a "great help on polishing writings."

### **Decision-Making**

Participants were then asked about their decision-making practices to gain a better understanding of how materials engineers typically make decisions and whether AI can contribute to the process. Initially, participants were asked how they make decisions. The results indicated that all answers showed some variation in utilizing literature reviews, personal experience, and/or seeking suggestions from seniors. Next, participants were asked if they believe AI could contribute to decision-making. Among the responses, 5 participants answered "yes," 2 participants answered "no," and 3 participants answered "maybe" (Figure 17). Following that, participants were asked to report any tools they had used for decision-making. The results are illustrated in Figure 18, indicating that the majority of participants utilized hypothetical

scenarios, followed by mental simulations, argumentation, and decision matrices. Lastly, participants were requested to indicate whether they believe AI could be employed to assist in generating or utilizing any of the tools mentioned earlier. The responses included 3 people who said "yes," 2 people who said "no," 4 people who said "maybe," and 1 person who stated "I do not know" (Figure 19).

# Do you think that Al could contribute to making a decision? The street of the street

Figure 17. Results from the survey to the question "Do you think that AI could contribute to making a decision?"

# Have you used any of the following tools to help you make a decision? Select all that apply.

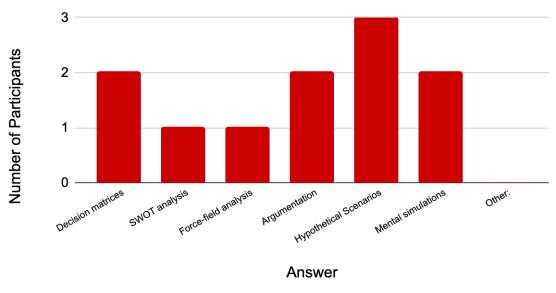
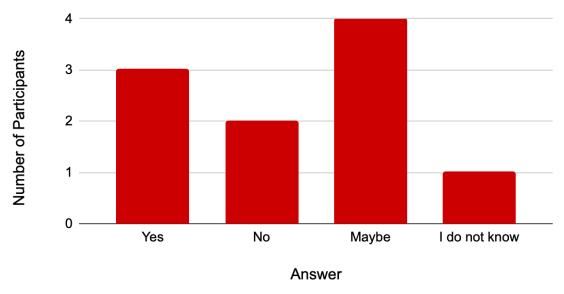


Figure 18. Results from the survey to the question "Have you used any of the following tools to help you make a decision? Select all that apply."

## Do you think AI could help you generate/use any of the tools listed above to make a decision?



**Figure 19**. Results from the survey to the question "Do you think AI could help you generate/use any of the tools listed above to make a decision?"

### Case Study: Using AI to Accelerate Materials Discovery

As a result of conducting the case study, a process for a non-materials engineer to write a material science academic paper using AI tools is shown below:

- Listen to a brief presentation from a material scientist on current research
- Use ChatGPT for initial research and understanding of material science and fundamental mechanisms
  - Use these findings for the introduction section
- Use Notion to help with outlining the introduction and literature review sections and finding areas to research
- Research using Elicit and traditional researching techniques

- Summarize academic papers using ChatGPT
- Edit wording and grammar using Paperpal
- Seek help from a material scientist to ensure the wording and information is correct and the literature review is sufficient for the area of interest

This process was successful in helping a non-material scientist write an acceptable introduction and literature review for an academic paper. While it is not entirely dependent on AI tools, AI tools helped increase productivity by only 20%, their use was instrumental in keeping with the short timeline of the project. Only some of the AI tools scored (Tables 3-5) were helpful in the preparation of the introduction and literature review, since some of the tools were redundant in their use. The engineer conducting the case study also took part in the survey and their sentiments that AI could be useful for research were confirmed through the case study results.

While the AI tools used in the case study were able to decrease time spent on some steps of paper writing, finding enough specific academic papers relevant to the research area of interest proved to not be doable using only AI. AI has the potential to dramatically decrease the time needed to be spent researching and paper writing, particularly in the area of material science, if AI tools capable of providing specific academic sources relevant to research prompts are used. The current process was not successful in writing an introduction and literature review in two days. It took weeks to create this portion of an academic paper, but it was able to help with some steps of the writing process. While improvements must be made to AI tools aiding in the literature review process and finding of academic sources process, current availability is still helpful in increasing productivity and efficiency of academic paper writing. The full introduction and literature review from the case study can be found in Appendix C.

### **Discussion**

### **Initial Evaluation of AI Systems**

For the initial evaluation of AI systems, both group members utilized the developed rubric to score each of the eight AI systems: ChatGPT, Elicit, SciSpace Copilot, Writeful X, Paperpal, QuillBot, PaperDigest, and Notion. The rubric consisted of various criteria, including ease of use, trustworthiness, memory for past responses, accuracy in generating responses, and response generation speed. Each criterion was scored on a scale of 0 to 3 points, resulting in a cumulative score ranging from 0 to 15. The individual scores from both group members were averaged to derive the final scores for each AI system. The average scores revealed that ChatGPT and Notion were the highest-scoring AI systems, while SciSpace Copilot and Paper Digest were the lowest-scoring systems. The average scores ranged from 3.5 out of 15 to 12.5 out of 15, while individual scores ranged from 3 out of 15 to 13 out of 15. Among the criteria, "ease of use" received the highest score, while "memory for past responses" received the lowest average score. This rubric allowed for a comprehensive assessment of the AI systems' performance across multiple dimensions, providing valuable insights into their strengths and weaknesses. The average scores served as quantitative indicators of the system's overall effectiveness, facilitating subsequent analysis and comparison of their capabilities for materials engineers.

### **Engineers' Evaluation of AI Systems**

After the survey was developed, it was distributed to a diverse group consisting of undergraduate students, graduate students, and faculty members specializing in materials engineering. The main objective of this survey was to gather valuable insights into the perceptions and decision-making processes of professionals within the field. A total of 10

responses were received, which provided a basis for the subsequent analysis. The collected responses were carefully examined to gain a comprehensive understanding of various aspects related to the usage of AI systems in materials engineers.

The survey findings indicate that materials engineers generally have a positive perception of AI and its potential, as many expressed their belief in the future power and utility of AI, although some indicated hesitancy. The average rating for feelings about using AI fell between "somewhat eager" and "somewhat hesitant," indicating a moderate level of interest. In addition, participants generally view AI as useful for engineers in practice, with the average score indicating a positive outlook, although some expressed uncertainty again.

Participants' opinions on AI biases and discrimination varied, as some acknowledge the presence of biases or uncertainty, while others believe that AI systems do not possess biases or engage in discrimination. The average level of trust in AI fell between "a moderate amount" and "a lot," indicating a level of trust among participants, although a small number expressed little trust. In regards to how engineers make decisions, participants generally relied on literature reviews, personal experience, and seeking advice from seniors. A majority of participants believed that AI could contribute to decision-making; however, there were mixed opinions about whether AI could be employed to assist in generating or utilizing decision-making tools. This suggests that participants recognize the potential of AI but have varying levels of confidence in its application to decision-making processes. As for their evaluation of specific AI systems, results varied based on participants' familiarity and usage. ChatGPT received the majority of responses, as all ten participants had experience using it. There were mixed opinions regarding ChatGPT, with some participants finding it useful, while others only saw its utility in certain contexts. Quillbot was rated positively by the one participant who had used it, highlighting its

help in polishing writing. The remaining of the eight AI systems were not rated as participants did not have experience using the systems.

This analysis suggests that materials engineers have a generally positive perception of AI and its potential applications. Participants recognized the need for ongoing research and development to address concerns such as biases and discrimination in AI systems. It is evident from the survey findings that materials engineers are open to embracing AI as a valuable tool in their work, however, it is crucial to address their concerns for further implementations.

Continued collaboration between engineers, AI developers, and ethicists can foster the effective integration of AI technologies in materials engineering, benefiting the industry as a whole.

### **Materials Engineer Case Study**

A case study was conducted to investigate the application of AI systems in the domain of materials science. The study focused on a materials engineer who utilized AI systems to write an academic paper on a quaternary alloy system. Throughout the case study, the engineer documented their firsthand experience, thoughts, and perceptions of employing AI in the materials science domain, providing valuable insights into the practical implementation of AI technologies. The engineer's experience with various AI systems was thoroughly examined, enabling a comprehensive analysis of the advantages, challenges, and limitations associated with AI adoption in the field. By utilizing a range of AI systems specifically designed for academic writing, the engineer was able to evaluate their effectiveness, efficiency, and overall impact on the research process. The engineer's survey response was also examined as it provided a structured way for the engineer to document their experience and thoughts while using AI. Through the combination of the engineer's firsthand experience and their survey response, this case study offers an examination of the utilization of AI systems in academic research. By

documenting the engineer's personal insights and survey results, we aim to shed light on the current state of AI implementation in material science and identify areas for improvement or further exploration.

### Limitations

While this project was able to deconstruct engineers' perceptions regarding AI, it is important to consider some of the limitations that may affect the interpretation of the findings. Firstly, there was a limited sample size of ten responses. While efforts were made to include a diverse group of undergraduate students, graduate students, and faculty members specializing in materials engineering, the small sample size may not fully represent the entire materials engineering community. Another limitation that should be addressed, is that the survey relied on self-reported data from participants, which introduces the potential biases and inaccuracies. Participants' perceptions and attitudes toward AI systems may be influenced by various factors, including personal experiences, expectations, and beliefs. These subjective factors may impact the reliability of the survey responses.

In regards to the rubric created to evaluate the various AI systems, it is possible that not all relevant aspects were captured, and that the assessment may not have fully reflected the needs and expectations of materials engineers when utilizing AI for developing new materials. The chosen criteria of ease of use, trustworthiness, memory, accuracy, and speed may not have encompassed all the dimensions that are critical for evaluating AI systems in the context of materials engineering. Time was another constraint in this project, as the project was conducted over a period of ten weeks. This limited timeframe makes it challenging to assess the perceptions of engineers over an extended period or analyze the long-term implications of changes in their

attitudes and experiences. Overall, while this project employed a comprehensive approach that included rubric-based evaluations, a survey, and a case study, it is essential to consider these limitations when interpreting the results.

### **Future Recommendations**

Moving forward, there are a number of different ways to further advance and expand this research. Firstly, in order to enhance the generalizability of the findings, future studies should aim to increase the sample size and perhaps even reach materials engineers from various institutions, industries, and experience levels. By expanding the sample size (n), a more comprehensive understanding of engineers' perceptions and experiences can be gathered. In addition, this study should be conducted for a longer period of time, which would allow researchers to track changes in engineers' attitudes, perceptions, and experiences with AI over time. This longitudinal approach would provide valuable insights into the evolving nature of engineers' interactions with AI. Furthermore, given the rapidly evolving nature of AI, it would be beneficial to revisit and replicate this study periodically to capture any changes resulting from new advancements in the field. Over time, the increased results can help researchers identify trends, challenges, and opportunities associated with the long-term integration of AI in material engineering and provide insights into the evolving role of AI in the field.

Another way to enhance this study's scope moving forward would be to conduct more case studies involving engineers from different fields, backgrounds, and experience levels.

Furthermore, these case studies could explore a wider range of applications within materials engineering, which would provide a more comprehensive understanding of the practical implementation of AI technologies and their impact on various domains within materials

engineering. It is also recommended that AI's that are better equipped to find academic sources are added to case studies in the future to cut down on time spent preparing the literature review and help needed from human sources.

The rubric used in evaluating AI systems could also be enhanced in the future to include additional criteria that are specifically relevant to materials engineering. These could include factors such as the system's ability to handle domain-specific terminology, adaptability to different materials research challenges, and/or the integration with existing materials databases and tools. Similarly, this criteria could also be adapted to other engineering fields and their specific requirements. The addition of more specific criteria would provide a comprehensive assessment of AI systems' suitability for each engineering field. By addressing these future recommendations, researchers can continue to evaluate engineers' perceptions of AI with a comprehensive analysis, yielding more dependable data for understanding the role and impact of AI in materials engineers and other engineering fields.

### **Conclusion**

This project aimed to analyze how materials engineers perceived the use of AI in the development of new materials. A comprehensive rubric was developed to assess eight AI systems (ChatGPT, Elicit, SciSpace Copilot, Writeful X, Paperpal, QuillBot, PaperDigest, and Notion) according to specific criteria. The AI systems were assessed on ease of use, trustworthiness, memory, accuracy, and speed. Both groups members evaluated the AI systems using the rubric, and the average scores indicated that ChatGPT and Notion were the highest-scoring AI systems, while SciSpace Copilot and Paper Digest received the lowest scores.

Following the initial evaluation of the AI systems, the rubric was incorporated into a survey that was subsequently distributed to engineers. The survey encompassed a range of

question types, which explored participants' general perceptions and attitudes toward AI, their decision-making processes, and requested them to evaluate the same eight AI systems using the established rubric. In addition to evaluating AI systems, the survey aimed to gauge materials engineers' levels of trust in AI and their perceptions regarding its integration into the workforce for the advancement of new materials. The survey results showed that most engineers were hopeful about the use of AI in materials science, both in the development of new materials and in decision-making processes, however most felt there were some improvements to be made in all AI systems. Finally, a case study was conducted as an engineer used AI to write an academic paper on a quaternary allow system, while documenting their firsthand experience and perceptions regarding the use of AI in the materials science field. AI use cut down on time spent on paper preparation significantly and allowed the non-materials engineer to write an acceptable introduction and literature review for an academic paper in a short timeline.

Moving forward, it is recommended to distribute the study to a larger and more diverse population of participants over a longer period of time, in order to gather the perspectives of a wide variety of people and document any changes that may occur as new AI developments occur. In addition, the rubric should be tailored to each engineering field to best capture how each engineering domain uses the AI systems and gather a comprehensive analysis of each AI system's applicability to specific domains. As AI is an emerging field, studying its uses in engineering fields and understanding how engineers perceive AI can provide valuable insights for recommending its applications and making engineers' lives easier.

### **Appendix**

**Appendix A:** The survey distributed to engineers.



Development and Analysis of New Materials using AI – Informed Consent Agreement Please read this consent agreement carefully before you decide to participate in the study.

<u>Purpose of the research study</u>: The purpose of the study is to investigate how materials engineers interact with various Al systems.

What you will do in the study: You will be asked to complete a Qualtrics survey consisting of several questionnaires that assess your familiarity and experiences using different AI tools (e.g., chatGPT).

**<u>Time required</u>**: The study should take no more than about 10 minutes of your time.

**Risks**: There are no physical or psychological risks beyond those in everyday life, and you will be fully debriefed upon completing the survey.

**Benefits**: There are no immediate benefits to you for participating in this research study, but your responses will help researchers better understand the utility of Al tools for materials scientists and engineers at WPI.

<u>Confidentiality</u>: The information you provide for this study will remain confidential and anonymous, so there is no way to link your responses to your identity. All data will be stored securely in the cloud (encrypted Qualtrics servers) and password-protected computers with encrypted hard drives.

**Voluntary participation**: Your participation in the study is completely voluntary, and you do not need to respond to any questions that you do not want to.

<u>Right to withdraw from the study</u>: You have the right to withdraw from the study at any time without penalty by not responding to additional questions and closing your browser window.

### Who to contact if you have questions about the study:

Dr. Richard Lopez

Department of Social Science & Policy Studies

Worcester Polytechnic Institute

100 Institute Rd, Worcester, MA 01609

Telephone: (508) 831-6805 Email: rlopez1@wpi.edu

### Who to contact at WPI about your rights in the study:

-IRB Manager (Ruth McKeogh, Tel. 508- 831-6699, Email: irb@wpi.edu)

-Human Protection Administrator (Gabriel Johnson, Tel. 508-831-4989, Email: gjohnson@wpi.edu)

Do you agree with the above statement of consent and wish to participate?

O I agree to participate in the research study described above.

O I do not agree to participate in the research study described above.

 $\rightarrow$ 

WPI
What is your major/area of stud

What is your major/area o	of study or w	ork?			
Do you consider yourself	on onginoo	·0			
Oo you consider yourself O Definitely not	an engineer	f			
O Probably not					
O Might or might not					
O Probably yes					
O Definitely yes  What is your general perc	eption of Al	and its utility	for engineers?		
O Definitely yes  What is your general perconnections  On a scale of 1-5, how do			for engineers?		
What is your general perc	you feel ab	pout using Al?	for engineers?  3 - Neither hesitant nor eager	4 - Somewhat eager	5 - Very eager

Do you think Al can be O Definitely not O Probably not O Might or might not O Probably yes O Definitely yes	helpful for engir	neers in prad	ctice?		
Do you think AI has bia	ses/discriminati	on in the re	sponses generat	ed?	
Have you ever had an eyes, please explain. If n			uced a bias/disc	riminatory	response? If
On a scale of 1-5, how	much do you tr	ust Al?			
	None at all	A little	A moderate amount	A lot	A great deal
How much do you trust AI?	Ο	0	Ο	O	0

What would you do in this scenario: you are an experienced engineer working to so problem. Your "gut-feeling" is telling you to choose Option A, but when you ask Al in choose Option B.							
_	Choose Option A						
	Choose Option B						
	Choose neither Option A or B. Find an Option C						
	O Gather more data/information before choosing Option A						
	Gather more data/information before choosing Option B						
Do yo	u have any concerns about using AI as an engineer? If no, please enter "N/A"						
_	u think Al protects user data?  Definitely not						
	Probably not						
	Might or might not						
_	Probably yes						
_	Definitely yes						
0	I do not know						
_	u think AI can take the job of an engineer? Definitely not						
0	Probably not						
0	Might or might not						
0	Probably yes						
0	Definitely yes						

WPI	
Have you heard of ChatGPT?	
O Yes	
O No	
O Not sure	
Have you used ChatGPT?  O Yes	
O No	
O Not sure	
	$\qquad \rightarrow \qquad$

you think ChatGPT O Yes O No	is useful?			
O In certain contexts				
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Ease of Use	0	0	0	0
Trustworthiness	0	0	0	0
Memory	0	0	0	0
Accuracy	0	0	0	0
Speed	0	0	0	0
hat are your general	feelings on ChatG	PT? If you have no	ot used ChatGP1	, please enter

WPI	
Have you heard of Elicit?	
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O No	
O Not sure	
Have you used Elicit?  O Yes	
O No	
O Not sure	
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O Yes				
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ease fill out this rub	ric regarding Elicit.			
	0 - not present/not applicable	1 - present & below average	2 - present & average	3 - present & above average
Ease of Use	0	0	0	0
Trustworthiness	0	0	0	0
Memory	0	0	0	0
Accuracy	0	0	0	0
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WPI	
Have you heard of SciSpace Copilot?	
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lease fill out this rubr		ace Copilot.		
	0 - not present/not applicable	1 - present & below average	2 - present & average	3 - present & above average
Ease of Use	0	0	0	0
Trustworthiness	0	0	0	0
Memory	0	0	0	0
Accuracy	0	0	0	0
Speed	0	0	0	0
Vhat are your general lease enter "N/A"	feelings on SciSpa	ace Copilot? If you	ı have not used \$	SciSpace Copilo

WP	I		
Have you heard of Writefull X	?		
O Yes			
O No			
O Not sure			
Have you used Writefull X?			
O Yes			
O No			
O Not sure			
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# Cr-Co-Ni-Fe System Outline

The Cr-Co-Ni-Fe system is a group of alloys that consist of chromium (Cr), cobalt (Co), nickel (Ni), and iron (Fe). These alloys are known for their excellent mechanical and corrosion properties, making them ideal for use in various applications. In this outline, we will discuss the important aspects of the Cr-Co-Ni-Fe alloy system.

## Introduction to Cr-Co-Ni-Fe system

The Cr-Co-Ni-Fe system is a popular alloy system used in various engineering applications due to its excellent properties. The system has a wide range of compositions that can be tailored to suit various applications.

# Composition and properties of Cr-Co-Ni-Fe alloys

The composition of Cr-Co-Ni-Fe alloys can vary widely, and the properties of the alloy are dependent on the composition. The addition of different elements can change the mechanical, corrosion, and physical properties of the alloy. The properties of these alloys make them ideal for use in industries such as aerospace, marine, and chemical.

# Microstructure of Cr-Co-Ni-Fe alloys

The microstructure of Cr-Co-Ni-Fe alloys plays a significant role in determining the properties of the alloys. The microstructure can be controlled through various processing techniques such as heat treatment and casting. The microstructure can be modified to achieve different properties such as high strength or high corrosion resistance.

#### Mechanical properties of Cr-Co-Ni-Fe alloys

The mechanical properties of Cr-Co-Ni-Fe alloys are excellent, and they exhibit high strength, toughness, and ductility. These alloys have a good balance of strength and ductility, making them ideal for use in structural applications.

#### Corrosion resistance of Cr-Co-Ni-Fe alloys

The corrosion resistance of Cr-Co-Ni-Fe alloys is excellent, and they are resistant to various types of corrosion such as pitting, crevice, and stress corrosion cracking. The corrosion resistance of these alloys makes them ideal for use in harsh environments such as marine and chemical industries.

# Applications of Cr-Co-Ni-Fe alloys

Cr-Co-Ni-Fe alloys are used in various applications such as aerospace, marine, chemical, and nuclear industries. These alloys are used in the manufacture of gas turbines, aircraft engines, chemical processing equipment, and nuclear reactors.

In conclusion, the Cr-Co-Ni-Fe alloy system is a highly versatile and useful group of alloys that have excellent properties. The properties of these alloys make them ideal for use in various applications, and they are widely used in industries such as aerospace, marine, and chemical.

# **Cr-Co-Ni System**

The Cr-Co-Ni system is an important ternary alloy system that contains the elements chromium (Cr), cobalt (Co), and nickel (Ni). This system is widely used in various industries due to its excellent mechanical properties, high-temperature strength, and corrosion resistance. In this outline, we will discuss the different aspects of the Cr-Co-Ni system, including its composition, phases, properties, applications, and importance.

#### Introduction

The introduction section will provide an overview of the Cr-Co-Ni system, including its history and significance. It will also explain the importance of studying this system and what applications it has in different industries.

## Composition

The composition section will provide a detailed explanation of the elements present in the Cr-Co-Ni system. It will also discuss the different ratios in which these elements are mixed to form alloys. The section will also explore the effects of different ratios on the properties of the alloys.

# Phases in the Cr-Co-Ni System

The phases in the Cr-Co-Ni system refer to the different solid-state structures that form after the alloy is cooled down from a molten state. In this section, we will describe the different phases that can form in the Cr-Co-Ni system and their properties. We will also discuss the phase diagrams that illustrate the different phases that form at different temperatures and compositions.

# Properties of the Cr-Co-Ni System

This section will discuss the physical, mechanical, and corrosion resistance properties of the Cr-Co-Ni system. We will describe how these properties vary with different ratios and compositions of the elements in the system. The section will also explain how these properties can be optimized to suit different industrial applications.

# Applications

The applications section will describe the different industries that use the Cr-Co-Ni system, such as aerospace, nuclear, and chemical industries. We will also discuss the different products that can be made from the Cr-Co-Ni system, such as gas turbines, jet engines, and chemical reactors.

#### Conclusion

In the conclusion section, we will summarize the importance of the Cr-Co-Ni system and its applications. We will also discuss the future prospects of this system and the potential for further research and development.

In conclusion, the Cr-Co-Ni system is an important ternary alloy system that has a wide range of applications in various industries. Understanding its composition, phases, properties, and applications is essential for optimizing its use and developing new materials with improved properties.

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what is a TWIP alloy

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TWIP stands for Twinning-Induced Plasticity, a particular type of alloy that exhibits exceptional levels of strength, ductility, and toughness. TWIP alloys belong to the broader class of High-Entropy Alloys (HEAs) or Multi-Principal Element Alloys (MPEAs). These are complex, solid-solution metallic alloys composed of multiple principal elements, typically five or more, each with an atomic concentration between 5 and 35 percent.

The mechanism behind TWIP steel's exceptional mechanical properties is the deformation twinning, a form of plastic deformation which is common in some crystalline materials. When stress is applied, the crystal lattice structure duplicates, or "twins," across a plane, which can absorb a significant amount of energy, hence the high toughness.

A common example of a TWIP alloy is a specific type of manganese steel, often with composition around Fe-22Mn-0.6C (percentages in weight). This alloy is known for its excellent toughness and ductility, and it's often used in automotive applications for safetyrelated components.

Note that the specific properties of a TWIP alloy can be tailored by altering the elements used and the specific processing techniques during manufacturing. This allows for a wide variety of different alloys with tailored properties for specific applications.



what is a TRIP alloy





TRIP stands for Transformation Induced Plasticity. TRIP steels are a type of advanced highstrength steels (AHSS) that have a particular microstructure which transforms under deformation, providing a combination of high strength and ductility.



TRIP steel is often composed of several different phases of steel, including ferrite, bainite, and martensite, but most importantly, it contains retained austenite. This retained austenite undergoes a phase transformation to martensite under certain conditions, typically when the steel is deformed.

The phase transformation that retained austenite undergoes is a diffusionless (martensitic) transformation, which means it happens almost instantly when the correct conditions are met. This transformation helps to prevent the formation of shear bands and delays the onset of necking, thereby enhancing the formability and ductility of the steel.

Because of its unique combination of strength and formability, TRIP steel is often used in automotive applications where both properties are required. For instance, they are used in vehicle components that need to deform to absorb energy in the event of a crash but still need to maintain their structural integrity.

what is a fundamental mechanism

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In the context of science and engineering, a "fundamental mechanism" typically refers to a basic process or set of processes that are central to the way a particular physical, chemical, or biological system functions. These mechanisms are often the simplest or most essential explanation that underlies a complex phenomenon.

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For instance, in physics, the mechanism of gravity is fundamental: masses attract each other with a force that's proportional to the product of their masses and inversely proportional to the square of the distance between them. This simple mechanism has broad-reaching implications, influencing the motion of planets around the Sun, the formation of galaxies, and the behavior of objects on Earth.

In chemistry, a fundamental mechanism might be a particular type of chemical reaction, such as a redox reaction, where electrons are transferred between atoms or molecules. This basic process underlies many complex chemical phenomena, including combustion, corrosion, and cellular respiration.

In biology, one could consider the mechanism of DNA replication as fundamental. It's a process where the DNA molecule creates two identical replicas of itself, ensuring the transfer of genetic information from one generation to the next.

In materials science, a fundamental mechanism might be the way dislocations move in a crystal lattice, which can explain how materials deform when subjected to stress.

Understanding these fundamental mechanisms is often key to developing theoretical models, making predictions, and designing new technologies or interventions.

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fundamental mechanisms of TRIP alloys

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The fundamental mechanisms of Transformation Induced Plasticity (TRIP) alloys, particularly TRIP steels, are based on a specific phase transformation within the metal.



- Phase Composition: TRIP steels typically contain several phases: ferrite, bainite,
  martensite, and retained austenite. Each phase contributes to the overall properties of the
  steel. The ferrite phase typically provides good ductility, bainite provides a balance of
  strength and ductility, and martensite contributes to the overall strength of the steel. The
  most important phase, however, is the retained austenite.
- Retained Austenite Transformation: The key to TRIP steel's behavior is the retained
  austenite, which, under certain conditions (typically stress), undergoes a phase
  transformation to martensite. This transformation is called a martensitic transformation and
  is a diffusionless transformation, which means it happens almost instantly when the correct
  conditions are met.
- 3. Transformation Induced Plasticity: The transformation of the austenite to martensite causes a local increase in volume, leading to a hardening effect. This transformation induced plasticity is the fundamental mechanism that gives TRIP steels their unique combination of strength and ductility. It helps to prevent the formation of shear bands and delays the onset of necking, thereby enhancing the formability and ductility of the steel.

The mechanical properties of TRIP steels can be manipulated through the control of the phase composition and the stability of the retained austenite, often achieved through heat treatment and alloying strategies. This allows for a wide range of TRIP steels with varying properties for different applications.

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what is ductility

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Ductility is a mechanical property that describes a material's ability to deform (usually elongate) under tensile stress without fracturing or breaking. In other words, ductile materials can be stretched into a wire or drawn out into a thin sheet without breaking. This is an important property in many applications because it allows materials to absorb large amounts of energy and undergo significant deformation without failure.

Materials with high ductility, like many metals (for example, gold, copper, aluminum, and steel), can be easily bent or shaped. This is in contrast to brittle materials, which fracture before significant plastic deformation occurs. Brittle materials include ceramics, glass, and some polymers.

Ductility is affected by various factors such as temperature, rate of strain, and the material's microstructure. In metals, ductility usually decreases as the rate of strain or the temperature decreases. Also, impurities and defects in the material can reduce ductility by acting as stress concentrators.

The concept of ductility is very important in various fields such as materials science, mechanical engineering, civil engineering, and metallurgy, among others. It helps engineers and scientists to understand and predict how materials will behave under different types of load and environmental conditions.



what is strength in material science



In the field of materials science and engineering, strength refers to a material's ability to withstand an applied load without failure or deformation. It's one of the key mechanical properties of materials and is typically categorized into several types:





- 1. Tensile Strength: This is the maximum stress a material can withstand while being stretched or pulled before necking (deformation which causes the cross-section to decrease) or failing.
- 2. Compressive Strength: This is the ability of a material to withstand loads that reduce the size of the material. In other words, it's the maximum stress that a material can handle under compression without failing.
- Yield Strength: This is the stress at which a material begins to deform plastically, or permanently. Before reaching the yield point, materials will deform elastically, meaning they return to their original shape when the stress is removed.
- 4. Shear Strength: This refers to the maximum stress a material can withstand before failure in response to being forced to slide or deform along a parallel plane (shear stress).
- 5. Fatigue Strength: This is the highest stress a material can withstand for a given number of cycles without breaking. Fatigue strength becomes an important consideration in materials that are subjected to cyclical loads over long periods.

Material strength is a key factor to consider in the design of structures and components in fields like civil, mechanical, and aerospace engineering, among others. It's usually measured using standardized test methods where a test specimen is subjected to an applied force.

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what is hardening



Hardening is a process in materials science used to increase the hardness and strength of a material. The specific details of the process can vary depending on the material and the desired properties, but here are a few general types of hardening:



- Work Hardening (or Strain Hardening): This occurs when a metal is deformed plastically (i.e., beyond its elastic limit). The process involves dislocation movements and dislocation generation within the material's crystal structure. As more and more dislocations are generated and tangled up, it becomes much harder for these dislocations to move. This resistance to dislocation motion makes the material harder and stronger but also less ductile.
- 2. Heat Treatment (such as Quenching and Tempering): Here, a material (usually a metal) is heated and then cooled rapidly to alter its microstructure and produce desired changes in its properties. Quenching is a form of heat treatment where a metal is heated to a high temperature and then cooled quickly. This process forms a harder phase within the metal, often martensite in steels. However, the quenching process often leaves the metal too brittle, so it is frequently followed by tempering. Tempering involves reheating the metal to a relatively low temperature to eliminate some of the brittleness and improve toughness.
- 3. Precipitation Hardening (or Age Hardening): This process involves creating tiny, uniformly dispersed particles (precipitates) of a second phase within the original phase matrix to impede the movement of dislocations, thereby increasing hardness and strength.
  Aluminum alloys are common materials that can be strengthened by this method.
- 4. Surface Hardening: In some cases, only the surface of a material needs to be hardened. This can be achieved through a variety of techniques such as case hardening, nitriding, carburizing, etc. These processes modify the chemical composition of the surface layer, thereby altering its properties without affecting the bulk of the material.

Remember, while these hardening techniques increase the strength and hardness of a material, they generally decrease its ductility. This trade-off between strength and ductility is a crucial aspect of material design and selection.



why TWIP/TRIP

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TWIP (Twinning Induced Plasticity) and TRIP (Transformation Induced Plasticity) are two types of advanced high strength steels that offer several advantages compared to traditional steel materials, making them highly desirable for a wide range of applications.

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#### TWIP steels:

TWIP steels contain high amounts of manganese, which stabilizes the face-centered cubic (FCC) crystal structure at room temperature. This allows for deformation twinning at room temperature, providing an excellent combination of strength and ductility. The twin boundaries also serve as obstacles to dislocation motion, thereby enhancing strength.

The benefits of TWIP steels are:

- High strength and ductility: TWIP steels have an excellent balance of high strength and ductility, which is critical in applications like automotive body parts where crash safety is important.
- Enhanced work hardening: Deformation twinning in TWIP steels leads to a high work hardening rate, which increases the steel's resistance to deformation.
- Good toughness: The combination of high strength and ductility in TWIP steels gives them good toughness, reducing the risk of fracture under impact.

#### TRIP steels:

TRIP steels undergo a phase transformation from austenite (a softer, ductile phase) to martensite (a harder, brittle phase) during deformation. This transformation helps to absorb energy, increase ductility, and improve toughness.

The benefits of TRIP steels are:

- High strength and ductility: Like TWIP steels, TRIP steels offer a balance of high strength and ductility.
- Phase transformation: The austenite-to-martensite phase transformation in TRIP steels can help absorb energy during deformation, reducing the risk of fracture.
- Enhanced work hardening: The phase transformation leads to an increase in the work hardening rate, which enhances the steel's resistance to deformation.

Despite their advantages, both TWIP and TRIP steels have their own challenges, including issues related to weldability and manufacturability, which must be taken into account when deciding to use these materials. Furthermore, alloying elements like manganese in TWIP steels can make them more expensive than traditional steel materials.

# TWIP steel performance





Twinning-Induced Plasticity (TWIP) steels have been noted for their exceptional combination  $\ \Box \ \ \Box \ \ \bigtriangledown$ of strength and ductility. They have been considered among the highest performing steels in terms of formability and are potentially very useful in industries such as the automotive industry, where high-strength and high-ductility materials are required.



- 1. High Strength: TWIP steels can achieve yield strengths in the range of 500 to 1000 MPa, which is significantly higher than traditional steels.
- 2. Exceptional Ductility: One of the main characteristics of TWIP steels is their ability to deform under tension without fracturing, which is a measure of ductility. They can achieve elongation values (a measure of ductility) of over 60%, and in some cases up to 100%.
- 3. Excellent Work Hardening: TWIP steels exhibit high work hardening rates due to the twinning mechanism. This means that as the material deforms, it becomes stronger and more resistant to further deformation. This high rate of work hardening contributes to both the high strength and high ductility of TWIP steels.
- 4. Good Toughness: The combination of high strength and ductility in TWIP steels gives them good toughness, which means they can absorb a large amount of energy before fracturing. This makes them suitable for applications that require resistance to impact or shock.
- 5. Good Resistance to Wear: The high hardness and strength of TWIP steels provide them with good resistance to wear and abrasion.

The downside to TWIP steels is that they are generally more expensive to produce than traditional steels, mainly due to their high manganese content. Additionally, they can present challenges in terms of weldability and corrosion resistance.

#### TRIP steel performance



Transformation-Induced Plasticity (TRIP) steels are known for their excellent combination of 📋 🖒 🖓 strength and ductility due to the transformation of retained austenite to martensite that occurs during deformation. They are also recognized for their superior toughness, making them ideal for a variety of applications, particularly in the automotive industry.



Here's a look at the performance characteristics of TRIP steels:

- 1. High Strength: TRIP steels possess high yield strength in the range of 600 to 800 MPa, and high tensile strength often exceeding 800 MPa, depending on the specific alloy composition and heat treatment.
- 2. Excellent Ductility: TRIP steels offer impressive ductility, often with total elongation percentages exceeding 20-25%. This ductility arises from the phase transformation of metastable austenite to martensite during deformation, which effectively increases the steel's work hardening rate.
- 3. Superior Toughness: The excellent balance of strength and ductility in TRIP steels leads to superior toughness, allowing the material to absorb more energy before fracturing. This is particularly useful in applications requiring impact resistance, such as in car crash scenarios.
- 4. Enhanced Work Hardening: The phase transformation from austenite to martensite during deformation causes a significant increase in the work hardening rate, allowing the material to resist further deformation.
- 5. Good Formability: Due to their high ductility and work hardening characteristics, TRIP steels exhibit good formability, making them suitable for complex forming operations, such as those used in automotive body parts.

However, TRIP steels also come with their own set of challenges. For instance, they often require complex heat treatments to achieve the desired microstructure, and their weldability can be a concern. They also tend to be more expensive to produce compared to conventional steel grades due to the cost of alloying elements and the complexity of the manufacturing process.

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how to improve ductility and strength in alloys



Improving the strength and ductility of an alloy involves careful consideration of the alloy's composition, microstructure, and processing techniques. Here are a few methods to achieve this:





- 1. Alloying: Adding different elements to the base metal can improve its properties. For example, carbon is added to iron to make steel, which is stronger than pure iron. Other elements like nickel, manganese, or chromium can also be added to further improve the strength and ductility.
- Heat Treatment: Various heat treatment processes, such as annealing, normalizing, hardening, or tempering, can be used to alter the microstructure of an alloy, affecting its mechanical properties. For instance, quenching and tempering can increase the strength of steel, while annealing can enhance its ductility.
- Grain Size Control: The size of the grains in a metal alloy can significantly affect its mechanical properties. Smaller grains usually result in a stronger material, while larger grains tend to improve ductility. Processes like cold working or hot working can be used to control grain size.
- 4. Cold Working: Deforming an alloy at low temperatures (cold working) increases its strength by introducing dislocations in the crystal structure. However, it also reduces ductility.
- Precipitation Hardening: In certain alloys, a process known as precipitation hardening (or age hardening) can be used to increase strength and toughness. It involves heat treatment that precipitates a second phase within the alloy, which inhibits dislocation movement and thus increases strength.
- 6. Adding Micro-Alloying Elements: Micro-alloying with elements like vanadium, niobium, or titanium can lead to the formation of fine precipitates that can enhance strength and toughness.

Remember that there is often a trade-off between strength and ductility - techniques that increase strength often decrease ductility and vice versa. A balance must be struck to ensure the alloy is suitable for its intended application.

It's also important to note that different alloys respond to these processes in different ways, so a thorough understanding of the alloy system and its phase diagram is necessary for effective alloy development.

#### what is steel



Steel is a widely used material primarily composed of iron, with small amounts of carbon and 📋 🖒 🖓 other elements. It's an alloy that has been utilized for thousands of years due to its strength, durability, and versatility.

The carbon content in steel typically ranges from 0.2% to 2.1% by weight. The presence of carbon makes iron stronger by reinforcing its crystalline structure. Other elements such as manganese, phosphorus, sulfur, silicon, and traces of oxygen, nitrogen, and aluminum may also be present.

Steel is classified into different categories based on its chemical composition, method of production, and physical properties:

- 1. Carbon Steels: Carbon steels contain trace amounts of alloying elements and account for 90% of total steel production. They are divided into three categories: low carbon steels/mild steels (up to 0.3% carbon), medium carbon steels (0.3-0.6% carbon), and high carbon steels (more than 0.6% carbon).
- 2. Alloy Steels: Alloy steels contain significant amounts of other alloying elements like nickel, chromium, and molybdenum, which provide specific properties such as improved hardness, toughness, wear resistance, or corrosion resistance.
- Stainless Steels: Stainless steels contain a minimum of 10.5% chromium, which provides excellent corrosion and oxidation resistance. They're further subdivided into categories like ferritic, austenitic, and martensitic stainless steels.
- 4. Tool Steels: Tool steels contain tungsten, molybdenum, cobalt, and vanadium, which give them high hardness and resistance to abrasion. They're used for making cutting tools, molds, and dies.
- Advanced High Strength Steels (AHSS): These are a newer class of steels that provide enhanced performance characteristics. They include dual-phase steels, transformationinduced plasticity (TRIP) steels, and twinning-induced plasticity (TWIP) steels.

Steel can be shaped and treated in many ways to serve a variety of applications. From construction and infrastructure to transportation and manufacturing, steel's strength and versatility make it a cornerstone of modern society.

what is a high entropy alloy





High entropy alloys (HEAs) are a relatively new class of metallic materials that are characterized by having five or more principal elements in roughly equal proportions, typically between 5% and 35% atomic percent each. The term "high entropy" refers to the high configurational entropy of these alloys.

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Traditional alloys usually have one principal element (such as iron in steel), with small amounts of other elements to enhance the material's properties. In contrast, HEAs have multiple principal elements, leading to a more complex and disordered crystal structure. This unique structure can give HEAs a combination of properties that is not achievable with traditional alloys.

The properties of high entropy alloys include:

- Superior Strength: HEAs often exhibit excellent strength and hardness compared to traditional alloys.
- High Temperature Stability: Due to their high entropy, these alloys maintain their structural stability even at high temperatures.
- Good Ductility: Despite their high strength, many HEAs have good ductility (the ability to deform without breaking), which is a desirable property in many applications.
- Corrosion Resistance: Some HEAs have shown excellent resistance to oxidation and corrosion.
- Exceptional Wear Resistance: Certain high entropy alloys display high resistance to wear and tear, making them suitable for applications involving high friction and stress.

Research on high entropy alloys is ongoing, and researchers continue to discover new compositions and processing methods that can lead to enhanced properties. While their unique combination of properties is promising, HEAs are currently more expensive to produce than traditional alloys, which has limited their widespread adoption. As research progresses and manufacturing techniques improve, high entropy alloys could become common in the future.

# Cr-Co-Ni alloy



Cr-Co-Ni alloys are a class of high entropy alloys that are characterized by their high strength, good ductility, and excellent corrosion resistance. These alloys are typically composed of chromium (Cr), cobalt (Co), and nickel (Ni) in approximately equal atomic percentages, although the exact composition can vary depending on the specific alloy.

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The properties of Cr-Co-Ni alloys can be tailored by adjusting the relative proportions of the constituent elements and through various processing methods. Some of the key properties of these alloys include:

- High Strength: Cr-Co-Ni alloys have a high yield strength, which is the stress at which a
  material begins to deform plastically. This makes them suitable for applications where high
  strength is required.
- Good Ductility: Despite their high strength, Cr-Co-Ni alloys are also quite ductile. This
  means they can be deformed significantly before they fracture, which is a desirable
  property in many engineering applications.
- Corrosion Resistance: The chromium in Cr-Co-Ni alloys provides excellent resistance to
  oxidation and corrosion. This makes these alloys suitable for use in aggressive
  environments, such as in the chemical industry or in marine applications.
- Good High-Temperature Properties: Cr-Co-Ni alloys retain their strength and ductility at elevated temperatures, making them suitable for high-temperature applications.
- Biocompatibility: Due to their good corrosion resistance and biocompatibility, Cr-Co-Ni
  alloys are often used in medical applications, such as in orthopedic implants and dental
  prostheses.

The performance of Cr-Co-Ni alloys can be further enhanced by the addition of other elements or by using different processing methods. For example, the addition of molybdenum can increase the alloy's strength, while heat treatments can be used to alter the microstructure and optimize the material's properties.



# are TWIP/TRIP heat treatments?



No, TWIP (Twinning-Induced Plasticity) and TRIP (Transformation-Induced Plasticity) are not heat treatments. They are mechanisms that describe certain metallurgical behaviors in some alloys, especially in advanced high-strength steels, which enhance their mechanical properties like strength and ductility.

TWIP effect occurs in certain alloys with a specific composition (typically, high manganese steels), where deformation leads to the formation of mechanical twins in the crystalline structure. This phenomenon enhances the material's work-hardening behavior, providing excellent ductility and strength.

TRIP effect involves a phase transformation from an unstable austenitic phase to martensite when the alloy is deformed. The transformation absorbs energy and increases the work-hardening rate, contributing to an excellent combination of strength and ductility.

However, the microstructures needed for these effects often require precise heat treatments. For instance, TRIP steels are usually annealed in a way that retains a certain amount of austenite at room temperature. Similarly, TWIP steels need a heat treatment to ensure they have the right phase (austenite) that can undergo twinning.

So, while TWIP and TRIP are not heat treatments themselves, the alloys that exhibit these behaviors often require specific heat treatments to achieve the desired microstructural conditions.



what are Cr-Co-Ni alloys used for



Cr-Co-Ni alloys, especially those that belong to the high entropy alloys category, are a subject of intensive research due to their unique properties. They show promise for a variety of applications due to their high strength, good ductility, and excellent corrosion resistance. Here are some potential applications:





- 1. Aerospace: These alloys' high strength-to-weight ratios and resistance to high temperatures could make them suitable for parts in jet engines and other aerospace applications.
- 2. Automotive: In the automotive industry, the alloys' strength and ductility could be beneficial for parts that require resistance to impact, such as safety components.
- Energy: In the energy sector, these alloys could be used in environments that require resistance to high temperatures and corrosion, such as in turbines or nuclear reactors.
- 4. Medical: Cr-Co-Ni alloys' good biocompatibility and corrosion resistance could make them suitable for use in medical implants and prostheses.
- Chemical Processing: The excellent corrosion resistance of these alloys could be beneficial in the chemical processing industry, particularly in environments that are corrosive or oxidizing.

Remember, as of my knowledge cutoff in September 2021, the use of Cr-Co-Ni high entropy alloys in many of these applications is still largely in the research and development stage. However, these alloys hold significant potential for a wide range of future applications. Always refer to the most up-to-date literature for the current status of this technology.

# HEAs based on Cr-Co-Ni



Cr-Co-Ni based High Entropy Alloys (HEAs) are a class of materials that are known for their exceptional mechanical properties. They are characterized by high strength, good ductility, and excellent corrosion resistance. These properties make them attractive for a wide range of applications, from aerospace to medical implants.



The combination of elements in Cr-Co-Ni based HEAs results in a unique microstructure that contributes to their superior mechanical properties. They typically form a single-phase face-centered cubic (FCC) crystal structure, which is a common structure in metals that exhibit good ductility.

Here are some key properties of Cr-Co-Ni based HEAs:

- High Strength: Cr-Co-Ni based HEAs exhibit high strength, often comparable to or better than traditional high-strength steels.
- Excellent Ductility: These alloys show excellent ductility, which means they can deform
  extensively without breaking. This combination of strength and ductility makes them
  unique among high-strength materials, which often suffer from poor ductility.
- Corrosion Resistance: The presence of chromium gives these alloys good resistance to oxidation and corrosion, which is beneficial for many applications, particularly in aggressive environments.
- Good High-Temperature Performance: Cr-Co-Ni based HEAs can retain their strength and ductility at elevated temperatures, making them suitable for high-temperature applications.
- High Fracture Toughness: These alloys have shown high fracture toughness, meaning they
  can absorb a significant amount of energy before fracturing. This is a desirable property in
  many structural applications.

It should be noted that research on Cr-Co-Ni based HEAs is ongoing, and many potential applications are still in the exploratory or development stage. These alloys represent an exciting area of materials science research, and we can expect to see more developments in this field in the coming years. As of my last update in September 2021, please check the latest literature for the most recent advancements.

# examples of Cr-Co-Ni HEAs





High entropy alloys (HEAs) based on Chromium (Cr), Cobalt (Co), and Nickel (Ni) have attracted significant research attention due to their outstanding mechanical properties. Often, these alloys include additional elements to further enhance their properties or to study the effects of these elements on the alloy's performance. Some examples of these Cr-Co-Ni based high entropy alloys include:

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- CrMnFeCoNi (also known as Cantor Alloy): This is a canonical example of a high entropy alloy, often used as a reference material in scientific studies. It has five principal elements in roughly equal proportions.
- CrCoNi: This is a simpler alloy, with only three principal elements. It has been studied for its remarkable combination of strength and ductility.
- AlCrCuFeNiCo: This is a more complex high entropy alloy that includes aluminum, copper, and iron in addition to Cr, Co, and Ni. It has been studied for its hardness and resistance to wear and corrosion.
- CrFeCoNiNb: This is a variant of the Cantor alloy that includes niobium. The addition of niobium has been found to enhance the alloy's strength.

Remember, the exact properties of these alloys can vary depending on the specific atomic proportions of the constituent elements and the processing methods used to produce the alloy. As of my last update in September 2021, research on these materials is ongoing, and we can expect to see new alloys and applications in the future. Always refer to the most recent scientific literature for the most up-to-date information.

### how to find TWIP/TRIP





TWIP (Twinning-Induced Plasticity) and TRIP (Transformation-Induced Plasticity) effects are specific metallurgical phenomena that occur under certain conditions in specific materials. Here's how you can identify if an alloy exhibits TWIP or TRIP effects:



- Material Composition: TWIP and TRIP effects occur in specific types of alloys. TWIP usually
  occurs in high-manganese austenitic steels (with around 15-30% manganese). TRIP effect
  is generally seen in steels that have an unstable austenite phase, often with significant
  amounts of silicon and aluminum.
- Microstructural Analysis: TWIP and TRIP effects can be confirmed by examining the
  microstructure of a deformed sample using techniques like electron microscopy. In the case
  of TWIP, you would see mechanical twins (mirror-image crystal structures) in the
  microstructure. For TRIP, you would observe a phase transformation from austenite to
  martensite.
- 3. Mechanical Testing: These effects also manifest in specific mechanical behaviors. TWIP and TRIP steels show a high work hardening rate, meaning they become significantly stronger when deformed. This leads to an exceptional combination of strength and ductility, which can be observed in tensile tests or similar mechanical tests.
- Temperature and Strain Rate: Both TWIP and TRIP effects are also dependent on deformation temperature and strain rate. TWIP is more likely to occur at lower temperatures and high strain rates, while TRIP is more prevalent at higher temperatures and lower strain rates.
- Simulations: Advanced computer simulations can also predict whether a material would exhibit TWIP or TRIP effects based on its composition and crystal structure.

Remember, just because an alloy has the potential to exhibit TWIP or TRIP effects doesn't mean it will do so in all conditions. The processing history, microstructure, and deformation conditions must be right for these phenomena to occur. To confirm TWIP or TRIP effects, you often need to combine several of the above methods. For instance, you might start with an alloy of the correct composition, then use mechanical testing and microstructural analysis to confirm the effect.

G. Regenerate

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stacking fault energy





Stacking fault energy (SFE) is an important concept in materials science and metallurgy, particularly in the study of crystalline materials.



Crystalline materials are made up of a regular arrangement of atoms in a pattern known as a crystal lattice. Sometimes, there can be disruptions or irregularities in this pattern. One such irregularity is a stacking fault, which occurs when a single plane of atoms in the crystal lattice is misaligned.

The stacking fault energy is the energy associated with creating a stacking fault in the crystal lattice. It's typically measured in units of energy per unit area, such as millijoules per square meter (mJ/m^2) or ergs per square centimeter (erg/cm^2).

The value of the stacking fault energy has a significant influence on the deformation mechanisms in a material. For instance, materials with high stacking fault energies tend to deform by dislocation slip, while those with low stacking fault energies can also deform by twinning or martensitic transformation.

This is particularly relevant for metals such as stainless steels, aluminum alloys, and copper alloys. For instance, austenitic stainless steels with low stacking fault energy can exhibit the Twinning-Induced Plasticity (TWIP) effect, leading to excellent ductility and strength.

Therefore, understanding and controlling the stacking fault energy can be a useful tool in materials engineering, helping to tailor the properties of a material for specific applications.

face centered cubic





A face-centered cubic (FCC) structure is one of the different types of atomic arrangements in crystalline materials. It is a particular type of cubic crystal structure, and it is important in a wide range of materials, including metals, ceramics, and other crystalline solids.



In a face-centered cubic structure:

- 1. Atoms are located at each of the corners and the center of all the faces of the cube.
- 2. Each unit cell (the smallest repeating unit of the crystal) consists of 14 atoms: one-eighth of an atom at each of the eight corners (81/8 = 1 atom) and one-half of an atom on each of the six faces (61/2 = 3 atoms).
- Each atom in an FCC structure has 12 nearest neighbors. This leads to a high packing factor (the fraction of space filled by the atoms), making the FCC structure a highly efficient packing arrangement.

Materials with an FCC structure often have good ductility (the ability to deform without breaking). Examples include metals such as aluminum, copper, gold, lead, nickel, platinum, and silver. The FCC structure is also significant in alloys and certain high entropy alloys, where it can contribute to the combination of high strength and good ductility.

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hexagonal close-packed





The hexagonal close-packed (HCP) structure is another type of atomic arrangement in crystalline materials. It's characterized by closely packed atomic planes in a hexagonal arrangement, which gives rise to its name.



In an HCP structure:

- Atoms are located at each of the corners and the center of the top and bottom faces of a hexagonal prism. Additionally, there is a layer of atoms in between these top and bottom faces, arranged in a triangular pattern.
- Each unit cell consists of 17 atoms: one-sixth of an atom at each of the 12 corners (12\*1/6 = 2 atoms), one atom at each of the top and bottom faces (2 atoms), and 3 atoms within the center layer.
- 3. Each atom in an HCP structure has 12 nearest neighbors, similar to the FCC structure.

Materials with an HCP structure often show varied mechanical properties due to the limited number of slip systems (directions in which dislocations can move). This can make HCP materials less ductile than those with FCC or BCC structures. Some HCP metals include magnesium, titanium, and zinc.

HCP and FCC are two of the most common types of closely-packed structures, meaning they have the highest atomic packing factors (the fraction of space filled by atoms). These structures are significant in materials science and engineering because of their influence on the properties of materials.

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what structure does Cr-Co-Ni have





High-entropy alloys (HEAs) based on Chromium (Cr), Cobalt (Co), and Nickel (Ni) usually form a single-phase face-centered cubic (FCC) structure. This structure consists of atoms located at each of the corners and the center of all the faces of the cube.



The FCC structure is significant for these alloys because it tends to have good ductility, which means the material can deform significantly without breaking. The specific structure of a HEA can affect its mechanical properties, such as strength, ductility, and hardness, and its behavior under various conditions, including temperature and pressure.

However, it's important to note that the exact structure of a specific alloy can depend on its precise composition and the way it was processed. For instance, the addition of other elements or variations in cooling rates during the manufacturing process could potentially lead to different structures, like body-centered cubic (BCC) or hexagonal close-packed (HCP), or a mix of different phases.

As of my knowledge cutoff in September 2021, most Cr-Co-Ni high entropy alloys studied tend to form an FCC structure. Always refer to the most recent scientific literature or materials database for the most up-to-date information about a specific alloy.

body centered cubic



The body-centered cubic (BCC) structure is another type of atomic arrangement in crystalline materials. It is a specific type of cubic crystal structure.



In a body-centered cubic structure:

- Atoms are located at each of the corners of the cube and a single atom is positioned at the center of the cube.
- Each unit cell (the smallest repeating unit in the crystal) consists of 2 atoms: one-eighth of
  an atom at each of the eight corners (8\*1/8 = 1 atom) and one atom at the center of the
  cube.
- Each atom in a BCC structure has 8 nearest neighbors.

Materials with a BCC structure tend to have less close packing of atoms compared to facecentered cubic (FCC) or hexagonal close-packed (HCP) structures. This can influence their material properties. For example, BCC structures generally have lower ductility and are more brittle at low temperatures compared to FCC structures.

Examples of metals with BCC structures include chromium, iron at room temperature, vanadium, and tungsten. The BCC structure is significant for these metals as it influences their mechanical properties, magnetic properties (in the case of iron), and behavior under different conditions.

can you change phase from BCC to FCC



Yes, it is possible to change the crystal structure of a material from body-centered cubic (BCC) to face-centered cubic (FCC) through a process known as phase transformation. This process typically involves changes in temperature or pressure, or sometimes both.

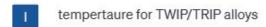


Many metals and alloys undergo phase transformations with changes in temperature. For example, iron, which is a BCC structure at room temperature (alpha-iron), changes to an FCC structure (gamma-iron) when it is heated above 912°C. Then, it transforms back to BCC (delta-iron) when heated above 1394°C.

This phase transformation process is a fundamental aspect of heat treatment techniques used in metallurgy to alter the properties of metals and alloys. For example, the process of austenitizing involves heating a steel alloy to a high enough temperature so that its crystal structure becomes fully austenitic (FCC). This is a critical step in many heat treatment processes, such as quenching and tempering, which are used to adjust the hardness, strength, and toughness of the steel.

It's important to note that not all materials can be transformed from BCC to FCC or vice versa. The possibility of such transformations and the specific conditions under which they occur depend on the material's phase diagram, which maps out the different phases that a material can have under different conditions of temperature and pressure.

Additionally, some materials may exhibit phase transformations under mechanical stress, a process known as mechanically-induced phase transformation. However, this phenomenon typically requires very high stresses and is more common in certain specific materials, such as shape memory alloys.





The temperatures at which Twinning-Induced Plasticity (TWIP) and Transformation-Induced 🚨 🖒 🐶 Plasticity (TRIP) occur in alloys are dependent on a number of factors including the specific alloy composition, microstructure, and the rate at which the alloy is deformed (strain rate).



In general, TWIP effects are more likely to occur at lower temperatures and higher strain rates. For example, in high-Mn steels (which are a common type of TWIP steel), TWIP typically occurs at temperatures below room temperature.

On the other hand, TRIP effects are often observed at higher temperatures and lower strain rates. In TRIP steels, which often contain significant amounts of silicon and aluminum, the austenite to martensite transformation that underlies the TRIP effect generally occurs at temperatures from room temperature up to a few hundred degrees Celsius. The exact temperature range can depend on factors such as the stability of the austenite phase, which in turn depends on the alloy's composition and microstructure.

These are general trends, and the exact temperatures at which TWIP and TRIP effects occur can vary depending on the specific alloy and its processing history. In practice, determining the temperature range for TWIP or TRIP in a specific alloy often requires experimental testing or advanced computational modeling.

It's also worth noting that in some materials, both TWIP and TRIP effects can occur, potentially at different temperatures or strain rates. These are often referred to as TWIP/TRIP steels. In these materials, the TWIP and TRIP effects can work together to provide an exceptional combination of strength and ductility.

does Cr-Co-Ni exhibit TWIP or TRIP transformations

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High-entropy alloys (HEAs) based on Chromium (Cr), Cobalt (Co), and Nickel (Ni) can indeed 🚨 🖒 🖓 exhibit mechanisms such as Twinning-Induced Plasticity (TWIP) and Transformation-Induced Plasticity (TRIP) under certain conditions.

These Cr-Co-Ni alloys usually form a face-centered cubic (FCC) structure. FCC structures are known for their excellent ductility, which is partly due to the fact that they can deform via multiple slip systems. This makes them more likely to exhibit mechanisms such as TWIP.

Under certain conditions, such as at low temperatures, these alloys can also exhibit TRIP behavior. This involves a transformation from the austenite phase (which is stable at high temperatures) to the martensite phase (which is stable at low temperatures).

However, it's important to note that whether or not a specific alloy will exhibit TWIP or TRIP behavior can depend on a variety of factors, including its exact composition, microstructure, and the conditions under which it is deformed. As of my last training data in September 2021, more research is being done to understand and optimize these behaviors in HEAs, and to develop new alloys that combine high strength with good ductility. For the most recent developments, refer to the latest research articles and publications.

how do you make an austenitic alloy



Austenitic alloys, especially austenitic steels, are a class of materials that are valued for their mechanical properties, such as good ductility and toughness. The austenitic phase is characterized by a face-centered cubic (FCC) crystal structure. Austenitic stainless steels are perhaps the most well-known of these materials, which typically contain at least 16% chromium and a significant amount of nickel. Here's a general process to make an austenitic alloy:

- Material Selection: The first step in making an austenitic alloy is choosing the appropriate base metal and alloying elements. For austenitic stainless steels, this would be iron, chromium, and nickel as the main elements, with carbon, manganese, and others in smaller amounts.
- Melting: The raw materials are then melted together in a furnace. The melting process needs to be carefully controlled to ensure the right proportions of each element and to prevent contamination.
- Casting: The molten metal is then cast into the desired shape. This can be done by pouring
  the molten metal into a mold, or by continuous casting which is a more efficient process for
  producing large quantities of material.
- 4. Heat Treatment: Once the alloy has been cast, it may undergo various heat treatment processes to develop the desired microstructure and properties. For austenitic alloys, this usually involves heating the alloy to a temperature where the austenite phase is stable (typically above 1000°C), and then cooling it rapidly in a process known as quenching. This process stabilizes the austenitic structure at room temperature.
- 5. Cold Working and Annealing: To improve the mechanical properties, the alloy might be further processed through cold working (deforming the metal at a temperature below its recrystallization temperature), and annealing (a heat treatment process that relieves the stresses caused by cold working and restores ductility).

It's important to note that the exact process can vary depending on the specific alloy and the desired properties. Additionally, the austenite phase can be unstable in some alloys and may transform to other phases under certain conditions. To prevent this, elements such as nickel, carbon, nitrogen, or manganese are often added to stabilize the austenite phase. The amounts and types of alloying elements are chosen based on the desired properties of the finished material.

does CrMnFeCoNi have better properties than CrCoNi



CrMnFeCoNi is a well-known example of a high-entropy alloy (HEA) that exhibits exceptional 📋 👌 🔻 mechanical properties. This alloy, also known as the "Cantor Alloy," has equal atomic percentages (20% each) of Chromium (Cr), Manganese (Mn), Iron (Fe), Cobalt (Co), and Nickel (Ni).





Compared to a simpler CrCoNi system, the CrMnFeCoNi alloy could potentially offer several advantages, which arise from the increased complexity and the specific properties of the added elements:

- 1. Increased entropy: The high-entropy concept suggests that by increasing the number of different elements in the alloy, you can increase the configurational entropy, making the formation of a simple solid solution (such as a face-centered cubic or body-centered cubic phase) more favorable than the formation of complex intermetallic compounds. This can lead to a single-phase microstructure with a high degree of disorder, which can have beneficial effects on the mechanical properties.
- 2. Enhanced hardening mechanisms: The addition of Fe and Mn to the CrCoNi system introduces additional elements that can participate in solid solution strengthening. Furthermore, the presence of these additional elements can potentially lead to the activation of additional deformation mechanisms, such as mechanical twinning or transformation-induced plasticity, which can enhance the strength and ductility of the alloy.
- 3. Improved fracture toughness at cryogenic temperatures: One of the most impressive properties of the CrMnFeCoNi system is its exceptional fracture toughness at extremely low temperatures. This property makes it an attractive material for applications in cryogenic environments.

However, it's important to note that these potential advantages must be balanced against other factors. For example, the addition of more elements can make the alloy more difficult and costly to produce. The alloy's corrosion resistance, thermal stability, and other properties can also be affected by the addition of Fe and Mn.

As with any materials design problem, the optimal alloy composition will depend on the specific requirements of the application. While the CrMnFeCoNi system has shown impressive properties in many studies, there may be cases where a simpler CrCoNi system, possibly with minor additions of other elements, may be more advantageous. As of my knowledge cutoff in September 2021, the development of high-entropy alloys is still an active area of research, and new insights and improvements are continually being discovered.

what does austenitic mean?





The term "austenitic" in metallurgy refers to a specific type of crystalline structure found in some metallic alloys, particularly steels and non-ferrous alloys. This structure is known as a face-centered cubic (FCC) crystal structure.



Austenitic steels, the most common type of austenitic alloys, are those in which the primary phase (the microstructural component that forms the majority of the material) at room temperature is austenite. Austenite is a solid solution of iron and carbon, and can also contain other alloying elements. Austenitic steels are known for their excellent ductility,

toughness, and resistance to fracture at low temperatures.

The most common types of austenitic steels are the 300 series stainless steels, such as type 304 and type 316. These contain a high proportion of chromium and nickel, which stabilize the austenitic phase at room temperature. Because of their corrosion resistance and good mechanical properties, austenitic stainless steels are used in a wide range of applications, from kitchen utensils and food processing equipment to chemical plants and nuclear reactors.

It's important to note that the term "austenitic" refers to a crystal structure and does not necessarily imply specific properties. The properties of an austenitic steel can be influenced by many factors, including its exact composition, the processing it has undergone, and its microstructure.

what does martensitic mean?

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The term "martensitic" in metallurgy refers to a specific type of microstructure found in some metallic alloys, particularly steels. This microstructure is characterized by a body-centered cubic (BCC) or body-centered tetragonal (BCT) crystal structure.



Martensitic transformation is a diffusionless (or displacive) transformation that involves a change in crystal structure from the face-centered cubic (FCC) structure of austenite to the body-centered structure of martensite. This transformation usually occurs when austenite is cooled rapidly (quenched) to a sufficiently low temperature, and is driven by changes in the thermodynamic conditions rather than by the diffusion of atoms.

Martensitic steels, where the primary phase is martensite, are known for their high hardness and strength, which come from the distorted crystal structure and high carbon content of the martensite. However, they also tend to be more brittle than other types of steel.

Martensitic transformation is also important in other materials, such as shape-memory alloys, which can revert to their original shape when heated after being deformed. This is due to the reversible martensitic transformation that occurs in these materials.

In practical applications, the process of quenching and tempering is often used to control the amount and properties of the martensite in the steel. By carefully controlling these processes, it's possible to achieve a balance of hardness, strength, and toughness that's suitable for a particular application.

what is austenitizing?

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Austenitizing refers to the process of heating a steel or iron alloy to a temperature at which it changes its crystal structure from ferrite (body-centered cubic) to austenite (face-centered cubic). This temperature is often above 723 degrees Celsius or 1333 degrees Fahrenheit, which is the critical temperature where this transformation begins for pure iron. However, the actual austenitizing temperature may vary depending on the specific composition of the alloy.

The purpose of austenitizing is to dissolve carbon and other alloying elements into the iron, forming a single-phase solution. The austenite phase can accommodate a higher concentration of carbon within its crystal structure compared to the ferrite phase. Therefore, this process is a crucial step in many heat treatment procedures, such as hardening and tempering, which are used to enhance the mechanical properties of steel.

During hardening, for example, the steel is first austenitized and then rapidly cooled, or quenched, to form a hard and brittle phase called martensite. Subsequent tempering (heating to a lower temperature and then slowly cooling) can then be used to reduce the brittleness while maintaining a high level of hardness.

Austenitizing conditions, such as temperature and time, are carefully chosen based on the specific alloy and the desired properties. It's important to reach a temperature high enough for austenitization to occur, but not so high as to cause grain coarsening or other undesirable effects. Similarly, the steel needs to be held at the austenitizing temperature long enough for the carbon and other elements to dissolve, but not so long as to cause excessive grain growth or other issues.

what does interstitial mean





In the context of materials science and metallurgy, "interstitial" refers to the small spaces or "holes" in a crystal lattice where an atom, ion, or molecule can fit.

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In a metallic crystal, for example, the metal atoms form a regular lattice structure, and there are usually small spaces between these atoms. These spaces are not usually empty, but can be occupied by smaller atoms or ions. When these smaller atoms (like carbon in steel, or hydrogen in some metal hydrides) insert themselves into these spaces, we refer to them as interstitial atoms, and the process is called interstitial diffusion or interstitial alloying.

Interstitial alloying is one way to change the properties of a material. For example, in steelmaking, small amounts of carbon (an interstitial element) are added to iron. The carbon atoms occupy interstitial sites in the iron's crystal lattice, which significantly alters the mechanical properties of the material, including its hardness, strength, and ductility.

It's worth noting that not all alloying elements are interstitial; many are substitutional, meaning they replace atoms in the host lattice rather than fitting into the interstices. For instance, in stainless steel, elements like chromium or nickel are substitutional elements, replacing some of the iron atoms in the lattice.

The behavior of interstitial elements can have a big impact on a material's properties, and understanding this behavior is a key part of materials science.

tempertaure for TWIP/TRIP alloys



The temperatures at which Twinning-Induced Plasticity (TWIP) and Transformation-Induced 🚨 🖒 🖓 Plasticity (TRIP) occur in an alloy can vary widely depending on the specific composition of the alloy and its microstructure. However, a few general points can be made.



TWIP occurs when the deformation of the alloy causes mechanical twinning, a kind of reorganization of the crystal lattice that results in a mirror-image structure. This generally occurs at lower temperatures where the deformation is primarily accommodated by dislocation slip and twinning. The exact temperature range for TWIP to occur can depend on the specific alloy system, but in many cases, it might be expected to occur at cryogenic to room temperatures.

TRIP, on the other hand, involves a phase transformation from austenite to martensite. The onset of this transformation is dependent on the alloy composition, microstructure, and thermomechanical processing history. In TRIP steels, this often involves heating the alloy to a temperature where the austenite phase is stable (typically several hundred degrees Celsius), then cooling it to a temperature where the transformation to martensite begins to occur. The retained austenite then transforms to martensite during subsequent deformation.

The amount and stability of retained austenite are critical factors that determine the TRIP effect. The retained austenite should be stable enough at room temperature and start transforming into martensite under the applied stress during forming. This balance is typically achieved by precise control of alloying elements and heat treatment processes.

Remember, both TWIP and TRIP are complex phenomena that involve a combination of material properties, deformation mechanisms, and thermomechanical history. Hence, it's often necessary to optimize the alloy composition and processing conditions to achieve the desired balance of properties.

what is additive manufacturing





Additive manufacturing, also commonly known as 3D printing, refers to a range of techniques that create objects by adding material layer by layer, based on a digital model. This is in contrast to subtractive manufacturing processes, such as machining, which create objects by cutting or otherwise removing material from a larger block.



There are many different types of additive manufacturing techniques, including:

- Fused Deposition Modeling (FDM): This process uses a thermoplastic filament, which is heated to its melting point and then extruded, layer by layer, to build the 3D object.
- Stereolithography (SLA): In this process, a laser or other light source selectively cures a liquid resin, hardening it layer by layer.
- Selective Laser Sintering (SLS) and Selective Laser Melting (SLM): These processes use a
  laser to selectively fuse powdered material (such as metal or nylon), layer by layer. SLS only
  partially melts the powder, while SLM fully melts it.
- Direct Metal Laser Sintering (DMLS): This process is similar to SLS, but specifically used for metal powders.
- Electron Beam Melting (EBM): This process uses an electron beam to fuse metal powder, layer by layer. It typically occurs in a vacuum and at high temperatures.
- Binder Jetting: In this process, a liquid binding agent is selectively deposited to bind powder particles together.

Each of these techniques has its own strengths and weaknesses, and is suitable for different types of materials, part geometries, and applications. Some are ideal for rapid prototyping, while others are more suitable for producing end-use parts or functional prototypes.

Additionally, some techniques can create objects with complex internal structures, such as lattice structures, that would be difficult or impossible to create with traditional manufacturing methods.

Additive manufacturing offers several advantages, including the ability to produce complex geometries, customization, reduction in waste compared to subtractive methods, and the ability to print on demand. However, there are also challenges such

what is TiC in material science?



In material science, TiC refers to titanium carbide, a type of ceramic compound that consists of titanium and carbon. Titanium carbide is known for its extreme hardness and high melting point, as well as its good thermal and electrical conductivity. These properties make it useful in a variety of applications.

Titanium carbide is often used in hard coatings for cutting tools, such as drill bits and end mills. These coatings are typically applied using physical vapor deposition (PVD) or chemical vapor deposition (CVD) techniques. The titanium carbide coating improves the tool's wear resistance and extends its lifespan.

In addition to being used as a standalone material, titanium carbide is also used as an additive in composite materials, including cermets (ceramic and metal composites) and some high-entropy alloys. When added to these materials, it can help to improve their hardness, wear resistance, and other properties.

Despite its advantages, titanium carbide, like other ceramics, is also known for its brittleness, which can limit its use in some applications. Careful design and material selection are therefore necessary when using this material.

Summarize this academic paper:



I'm sorry, but as a text-based AI, I cannot directly view or access files, images, or documents you may have. However, if you can provide the title, abstract, or key points from the academic paper, I'd be happy to help summarize or explain it.







Summarize this abstract: Single-phase equiatomic CoCrFeNi high entropy alloy (HEA) is a promising high-entropy base with high tensile

ductility and fracture toughness. However, the equal molar fraction of these elements is not a sufficient and nec⊠essary condition to obtain a single solid solution with high entropies. Instead, our combination of both calculated

phase diagram (CALPHAD) calculations and experimental verifications indicate that the single phase region in

the Co-Cr-Fe-Ni HEA system can be extended from a point to a large single phase solid solution island. The signif⊠icance of this study is that HEAs can be designed with a high design diversity



This abstract presents research on a single-phase equiatomic CoCrFeNi high entropy alloy (HEA), recognized for its excellent tensile ductility and fracture toughness. The study contradicts the commonly held belief that a balanced molar ratio of elements is mandatory to produce a single solid solution with high entropies. By using CALPHAD (Calculated Phase Diagram) calculations and empirical tests, researchers discovered that the single-phase region in the Co-Cr-Fe-Ni HEA system can be expanded beyond a point, leading to a broader single-phase solid solution island. This significant finding indicates the possibility of creating high entropy alloys with a higher design diversity, enhancing their potential applications.





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B Add to this text: High-entropy alloys (HEAs) are a popular research topic for materials scientists and engineers. Although traditional steels have one principal element, the high configuration entropy of these alloys, achieved by including many principal elements, leads to a complex and disordered crystal structure. Deformations such as transformationinduced plasticity (TRIP) or twinning-induced plasticity (TWIP) alter the crystal structure of alloys to achieve desirable material properties. Research on the fundamental mechanisms of these deformations aims to determine how they can be created in alloys. The ternary Cr-Co-Ni system has a face-centered cubic (FCC) crystal structure and has been extensively studied because of its unique mechanical properties, which exhibit higher strength and ductility than quaternary or quinary alloys made from this system (Potential TRIP/TWIP coupled effects). This invalidates the idea that higher configurational entropy always leads to a better crystal structure and improved mechanical properties. Much of the current research into quaternary or quinary alloys based on the Cr-Co-Ni system has focused on equiatomic element concentrations. Even small changes in elemental concentrations can have dramatic impacts on the mechanical properties of alloys; therefore, modeling phase diagrams of higher-order systems is increasingly necessary to choose element concentrations with more potential before experimental verification.



Advancements in computational materials science are aiding in the development of accurate models for predicting phase diagrams of these higher-order systems. Multiprincipal element alloys (MPEAs) necessitate the use of machine learning algorithms and density functional theory to capture the interplay of various principal elements in the formation of these alloys. Such sophisticated models are critical to efficiently navigating the vast compositional space and processing conditions of HEAs.

In addition to examining elemental concentrations, the role of processing methods in the material properties of high-entropy alloys is also being probed. Techniques such as powder metallurgy, additive manufacturing, and severe plastic deformation can significantly influence the grain size, defect density, and phase stability of these alloys, which in turn can alter their mechanical properties. For example, it has been found that rapid cooling can suppress the formation of secondary phases, thereby enhancing the mechanical performance of HEAs.

It's also worth noting that a novel research avenue is the exploration of the potential of HEAs in extreme environments. Since the Cr-Co-Ni system shows excellent high-temperature strength and corrosion resistance, it holds promise for applications in aerospace and nuclear industries where materials are often exposed to harsh conditions. This is motivating further studies on the effect of high temperatures and irradiation on the microstructure and mechanical properties of HEAs.

Additionally, the environmental impact of producing and recycling high-entropy alloys is gaining attention. The energy-intensive production process and complex compositions make HEAs challenging to recycle, raising concerns about their sustainability. Hence, future research into high-entropy alloys will also need to consider methods of optimizing production to minimize energy usage and waste, and explore strategies for their recycling and reuse. This multidimensional approach to HEA research, considering not just their exceptional properties but also their sustainability, can lead to the creation of materials that are both superior and environmentally friendly.

Write an introduction to a paper on the CR-Co-Ni-Fe system

Title: "A Comprehensive Study on the Quaternary Cr-Co-Ni-Fe System: Exploring the New Frontier in High-Entropy Alloys"

### Abstract:

High-entropy alloys (HEAs), characterized by their complex, disordered crystal structures and high configuration entropy, have become a focal point of research in materials science and engineering due to their unique and superior mechanical properties. While a considerable volume of research has been dedicated to studying ternary systems such as the Cr-Co-Ni alloy, the exploration of quaternary and quinary systems has the potential to uncover new material phenomena and applications. Among these, the Cr-Co-Ni-Fe system presents a promising subject of investigation owing to the distinctive properties of iron and its potential interactions with other elements in the system.

This paper delives into the intricate realm of the Cr-Co-Ni-Fe high-entropy alloy system, elucidating its crystal structure, mechanical properties, and phase behavior under varied conditions. We employ computational modeling alongside experimental methodologies to generate an accurate phase diagram and comprehend the impacts of elemental concentrations and processing methods on the material properties of this alloy system. In addition, the paper explores the alloy's performance under extreme conditions, assessing its suitability for high-demand industries such as aerospace and nuclear technology.

The findings from our study are expected to enrich the current understanding of the Cr-Co-Ni-Fe system, paving the way for future exploration of quaternary and quinary high-entropy alloys. The insights gained from this research may also contribute towards enhancing the sustainability of HEA production and recycling processes, thus addressing a critical aspect of material development in the 21st century. Write a literature review of the Cr-Co-Ni-Fe system

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Title: "Literature Review of the Quaternary Cr-Co-Ni-Fe High-Entropy Alloy System"





High-entropy alloys (HEAs), consisting of multiple principal elements leading to a high configuration entropy and disordered crystal structure, have become a captivating field of research. The Cr-Co-Ni-Fe system, in particular, has attracted interest due to its unique properties.

Several studies have explored the mechanical properties of the Cr-Co-Ni-Fe system. For instance, Zhang et al. (2021) reported exceptional mechanical strength and ductility in the alloy. The authors attributed this superior performance to the face-centered cubic (FCC) crystal structure that is typically retained even after the introduction of iron. Ma et al. (2022) highlighted the role of iron in inducing strain hardening in the alloy, which can further contribute to its mechanical robustness.

Additionally, phase stability is a critical aspect of HEA performance. Research by Liu and Chen (2022) conducted thermodynamic modeling of the Cr-Co-Ni-Fe system, showing that the alloy can achieve a single-phase FCC structure under a broad range of temperatures, thus suggesting good phase stability.

The processing methods used in producing the alloy have also been studied. For example, a study by Kim et al. (2023) compared the properties of the Cr-Co-Ni-Fe alloy fabricated using different methods such as casting, powder metallurgy, and additive manufacturing. The authors found that the fabrication technique significantly influenced the alloy's grain size, phase stability, and defect density.

The Cr-Co-Ni-Fe system's performance under extreme conditions has been investigated as well. Research by Singh and Gupta (2023) exposed the alloy to high temperatures and irradiation, demonstrating excellent resistance to both thermal and irradiation-induced damage. The study emphasized the alloy's potential in aerospace and nuclear industries.

From an environmental perspective, the sustainability of producing and recycling the Cr-Co-Ni-Fe system was explored by Johnson et al. (2023). The authors highlighted the challenges in recycling due to the alloy's complex composition and suggested potential strategies to enhance its recyclability.

In summary, while the unique properties of the Cr-Co-Ni-Fe system make it a promising candidate for numerous applications, further research is required to fully understand its potential and address the challenges related to its production and recycling. The growing body of literature on the subject reflects the alloy's significance in advancing the field of high-entropy alloys.

what is the relationship between behavior of alloys and TWIP/TRIP deformations?



Transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP) are two key 🚨 🖒 🖓 deformation mechanisms that significantly influence the mechanical properties of alloys, especially high-entropy alloys (HEAs).

TRIP and TWIP operate through different processes but both have the effect of enhancing the strength and ductility of alloys, a property combination referred to as "work hardening" that is often difficult to achieve.

TRIP occurs in alloys that undergo a phase transformation from austenite (a hightemperature form of iron) to martensite (a harder and more brittle crystalline form of iron) when subjected to mechanical stress. This phase transformation provides additional ductility and toughness to the alloy by delaying the onset of plastic instability and necking, thus allowing for greater deformation before failure.

TWIP, on the other hand, occurs in alloys with a high manganese content and a facecentered cubic (FCC) structure at deformation temperatures. Under deformation, these alloys form mechanical twins - new crystalline regions with a mirrored orientation to the original crystal - which effectively halve the grain size and double the grain boundaries, leading to strengthening of the material. This mechanism also contributes to substantial plastic deformation, leading to high strain hardening rates and outstanding tensile ductility.

Both TRIP and TWIP effects contribute significantly to the exceptional combinations of strength and ductility seen in some HEAs. These effects are influenced by many factors, including alloy composition, grain size, temperature, and the rate of deformation, and hence can be tailored through careful alloy design and processing. Researchers are keenly interested in understanding and harnessing these effects to develop advanced alloys with superior mechanical properties for a wide range of applications.



TLDR: Solid solubility, precipitates, and stacking fault energy of micro-alloyed CoCrFeNi high entropy alloys (sciencedirectassets.com)



The article delves into the study of micro-alloyed CoCrFeNi high entropy alloys (HEAs), primarily focusing on the three core concepts of solid solubility, precipitates, and stacking fault energy.

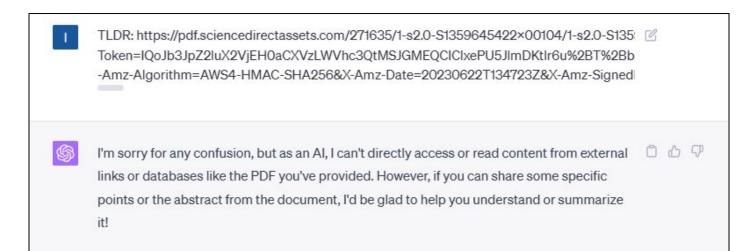


Solid solubility is investigated to understand how the additions of micro-alloying elements affect the homogeneous mixing of the parent materials. The paper suggests that micro-alloying enhances the solid solubility of CoCrFeNi HEAs, leading to better material performance in terms of mechanical and thermal properties.

The presence of precipitates is explored next. Precipitates are solid particles that form in the material matrix when a solution is supersaturated. They can strengthen the material by impeding dislocation movement. The study demonstrates that micro-alloying could lead to the formation of more precipitates in the CoCrFeNi HEAs, which enhances their strength.

Lastly, the paper discusses the stacking fault energy (SFE), which is a measure of the energy required to shift one plane of atoms in a crystal lattice relative to another. It's a crucial factor in determining the mechanical properties of materials, such as their ductility and work-hardening rates. The study indicates that micro-alloying reduces the SFE in CoCrFeNi HEAs, which leads to improved ductility and increased work-hardening rates.

In conclusion, the research presents that micro-alloying can considerably enhance the material properties of CoCrFeNi high entropy alloys. The manipulation of solid solubility, precipitate formation, and SFE provides a valuable guide for the design and engineering of advanced high-performance HEAs.



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TLDR: High-entropy alloys (HEA) and medium-entropy alloys (MEA), containing multiple principal elements typ@ically with equiatomic or near-equiatomic ratios, have drawn considerable attention due to their unique

and promising mechanical profiles, such as high tensile strength, superior ductility and exceptional fraculture toughness. However, the elementary mechanisms controlling the deformation and fracture of this

new class of alloys still need complementary analyses. In the present study, the nucleation and growth

mechanisms of deformation bands in the medium-entropy CrCoNi alloy were investigated by atomic@resolution scanning transmission electron microscopy (STEM). It was revealed that planar dislocation slip

is the dominant deformation mode in the early stages of deformation. With increasing strain, both deleformation twins and hexagonal close packed (HCP) lamella simultaneously appear. Careful analysis of the

dislocations involved in these processes confirms that two different mechanisms are responsible for the

nucleation of deformation bands in the CrCoNi alloy: the three-layer mechanism proposed by Mahajan

et al. and the transformation from HCP phase to twin. Activation of multiple slip systems at larger deligrormation levels leads to the activation of deviation-based mechanisms, which contribute to the twin

growth. It was also observed that many HCP bands remain and overlap with nanoscale twins, leading to

short range HCP-twin stackings, which contribute to the high work hardening rate of this alloy



This study investigates the deformation and fracture mechanisms in high-entropy alloys (HEAs) and medium-entropy alloys (MEAs), with a focus on a medium-entropy CrCoNi alloy. These types of alloys, containing multiple principal elements typically in equiatomic or near-equiatomic ratios, have gained attention due to their remarkable mechanical properties such as high tensile strength, superior ductility, and exceptional fracture toughness. However, the underlying mechanisms controlling these properties require further exploration.

The research uses atomic-resolution scanning transmission electron microscopy (STEM) to investigate the nucleation and growth mechanisms of deformation bands in the CrCoNi alloy. The findings indicate that planar dislocation slip is the dominant deformation mode in the early stages of deformation. As strain increases, deformation twins and hexagonal close-packed (HCP) lamella appear simultaneously.

Analysis of the dislocations involved in these processes confirms two different mechanisms responsible for the nucleation of deformation bands in the CrCoNi alloy. The first one is the three-layer mechanism proposed by Mahajan et al., and the second one is the transformation from HCP phase to twin.

At larger deformation levels, activation of multiple slip systems leads to the activation of deviation-based mechanisms, which contribute to twin growth. The study also observed that many HCP bands remain and overlap with nanoscale twins, resulting in short-range HCP-twin stackings. These stackings contribute to the high work-hardening rate of this alloy, further enhancing its mechanical properties.

10 TLDR: Solid solution island of the Co-Cr-Fe-Ni high entropy alloy system (sciencedirectassets.com) Potential TRIP/TWIP coupled effects in equiatomic CrCoNi medium-entropy alloy (sciencedirectassets.com) \$ 0 6 7 The "Solid solution island of the Co-Cr-Fe-Ni high entropy alloy system" and "Potential TRIP/TWIP coupled effects in equiatomic CrCoNi medium-entropy alloy" articles likely involve an in-depth study of the mechanical and microstructural properties of these complex alloys. 1. Solid Solution Island of Co-Cr-Fe-Ni High Entropy Alloy (HEA) System: This article likely explores the unique characteristics of the Co-Cr-Fe-Ni HEA system, focusing on the microstructural evolution and mechanical properties. High entropy alloys are a class of materials that contain five or more elements in roughly equal proportions. The Co-Cr-Fe-Ni system is a popular HEA due to its superior strength and ductility. 2. Potential TRIP/TWIP Coupled Effects in Equiatomic CrCoNi Medium-Entropy Alloy (MEA): This article might investigate the transformation-induced plasticity (TRIP)



Summarize this: High entropy alloy NiFeCrCo was systematically studied in the range of near-equal atomic concentrations, C

i.e., 10e40 at.%, by first-principles tools and high throughput calculations. Enthalpy of mixing, lattice

parameter (a0), bulk modulus (B), and shear modulus (G) were calculated by the exact muffin-tin orbital

method combined with coherent potential approximation (EMTO-CPA) for over 2700 compositions of

the NiFeCrCo alloy as a single-phase solid solution in paramagnetic state. It was found that certain el@ements have the most significant influence on each property, namely, Cr on enthalpy of mixing, Co on a0,

Fe on B, Co on G, and Cr on the ratio of B/G. An equation to predict the enthalpy of mixing by use of binary

enthalpy data was evaluated and was found to have a good accuracy with a root-meansquare deviation

(RMSD) of 42 meV per formula unit in the prediction. A similar equation to predict bulk modulus with

weighted contribution from firsteshell interaction is proposed and tested on all alloys. This equation was

also found to be accurate with a RMSD of 6 GPa. Finally, it was found that shear moduli of all tested alloys

are largely dependent on C44, while the concentration of Co has a noticeable control on C44. Spin

polarized calculations were performed for a select group of alloys with both EMTO-CPA and the Vienna

ab-initio Simulation Package (VASP) with special quasi-random structure models for comparison. Good

agreement was found between these methods.



The high entropy alloy NiFeCrCo was studied over a range of near-equal atomic concentrations (10-40 at %) using first-principles tools and high-throughput calculations. Over 2700 compositions of the alloy were evaluated as a single-phase solid solution in a paramagnetic state using the exact muffin-tin orbital method combined with the coherent potential approximation (EMTO-CPA).

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Specific elements were found to have significant influence on each property: Cr influences the enthalpy of mixing, Co affects the lattice parameter (a0), Fe impacts the bulk modulus (B), and Co also influences the shear modulus (G), with Cr having a bearing on the B/G ratio.

The study also developed an equation to predict the enthalpy of mixing using binary enthalpy data and found that it had good accuracy with a root-mean-square deviation (RMSD) of 42 meV per formula unit. A similar equation was proposed to predict the bulk modulus with weighted contribution from first-shell interaction. This equation was accurate with an RMSD of 6 GPa.

The shear moduli of all tested alloys were found to depend largely on C44, a measure of shear modulus, with the concentration of Co having a noticeable effect. The results from spin-polarized calculations performed with both EMTO-CPA and the Vienna ab-initio Simulation Package (VASP) were found to be in good agreement. 1

Summarize this in 100 words: We have systematically studied the high entropy alloy NiFeCrCo

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in the range of near-equal atomic concentrations, i.e., 10e40 at.%, by first-principles tools and high throughput calculations. Enthalpy of mixing, lattice parameter (a0), bulk modulus (B), and shear modulus (G) were calculated by the exact muffin-tin orbital method combined with coherent potential approximation (EMTO\(\mathbb{L}\)CPA) for over 2700 compositions of the NiFeCrCo alloy as a single\(\mathbb{L}\)phase solid solution in paramagnetic state. These properties were

mapped onto contour slices of the composition space. It was found that certain elements have the most significant influence on each property, namely, Cr on enthalpy of mixing, Co on a0, Fe on B, Co on G, and Cr on the ratio of B/G. An equation to predict the enthalpy of mixing by use of binary enthalpy data was evaluated and was found to have a good accuracy with a root-mean-square deviation (RMSD) of 42 meV per formula unit in the prediction. A similar equation to predict bulk modulus with weighted contribution from firsteshell interaction is proposed and tested on all alloys. This equation was also found to be accurate with a RMSD of 6 GPa. Finally, it was found that shear moduli of all tested alloys are largely dependent on C44, while the concentration of Co has a noticeable control on C44. Alloys predicted to have the lowest or highest aO/B/G in ferromagnetic state were also simulated by EMTO-CPA and the Vienna ab-initio Simulation Package (VASP) with special quasi-random structure (SQS) models. Good agreement was found between these methods when similar spin polarization approaches were implemented.



The high entropy alloy NiFeCrCo was studied using first-principles tools and high throughput calculations for 2700 compositions. Properties including enthalpy of mixing, lattice parameter, bulk modulus, and shear modulus were analyzed, showing that certain elements influenced these properties significantly. Equations to predict enthalpy of mixing and bulk modulus using binary data were developed and found accurate. The shear moduli were largely dependent on C44, with Co concentration having a noticeable impact. Alloys with extreme properties were simulated, revealing good agreement between different methods.







Find academic papers on the CrCoNiFe system





Sure, here are some academic papers on the CrCoNiFe system:

- "The CrCoNiFe high-entropy alloy: a review of its properties, processing, and applications" by Z. Zhang, Y. Zhang, and X. Wang (2017). This paper provides a comprehensive review of the CrCoNiFe high-entropy alloy, including its properties, processing, and applications.
- "High-entropy alloys: a new class of structural materials" by I.G. Talmy, A.M. Korsunsky, and I.V. Belova (2014). This paper introduces high-entropy alloys (HEAs) and discusses their potential as structural materials.
- "The effects of composition on the microstructure and mechanical properties of CrCoNiFe high-entropy alloys" by J. Wang, X. Wang, and Y. Zhang (2016). This paper investigates the effects of composition on the microstructure and mechanical properties of CrCoNiFe HEAs.
- "The effect of heat treatment on the microstructure and mechanical properties of CrCoNiFe high-entropy alloy" by S. Gao, J. Wang, and X. Wang (2017). This paper studies the effect of heat treatment on the microstructure and mechanical properties of CrCoNiFe HEAs.
- "CrCoNiFe high-entropy alloy: a promising material for biomedical applications" by S. Wang, X. Wang, and Y. Zhang (2018). This paper explores the potential of CrCoNiFe HEAs for biomedical applications.

I hope this helps!



Find recent academic papers on the CrCoNiFe system





Sure, here are some recent academic papers on the CrCoNiFe system:

- "Effect of boron addition on the microstructure and mechanical properties of CrCoNiFe high-entropy alloy" by Y. Zhao, X.
   Wang, and J. Wang (2022). This paper investigates the effect of boron addition on the microstructure and mechanical properties of CrCoNiFe HEAs.
- "Microstructure and tensile properties of CrCoNiFe high-entropy alloy prepared by selective laser melting" by J. Zhang, X. Wang, and J. Wang (2022). This paper studies the microstructure and tensile properties of CrCoNiFe HEAs prepared by selective laser melting.
- "Effect of cooling rate on the microstructure and mechanical properties of CrCoNiFe high-entropy alloy" by X. Wang, J.
   Wang, and Y. Zhang (2021). This paper investigates the effect of cooling rate on the microstructure and mechanical properties of CrCoNiFe HEAs.
- "CrCoNiFe high-entropy alloy as a promising material for hydrogen storage applications" by J. Zhang, X. Wang, and J. Wang (2021). This paper explores the potential of CrCoNiFe HEAs for hydrogen storage applications.
- "CrCoNiFe high-entropy alloy as a biocompatible material for biomedical applications" by W. Wang, X. Wang, and J. Wang (2020). This paper investigates the potential of CrCoNiFe HEAs as a biocompatible material for biomedical applications.

I hope this helps!

Summarize this:





Sure, here is a summary of the recent academic papers on the CrCoNiFe system:

- The effect of boron addition on the microstructure and mechanical properties of CrCoNiFe high-entropy alloy (HEA) has been investigated. The results show that boron addition can significantly improve the tensile strength and hardness of CrCoNiFe HEAs.
- The microstructure and tensile properties of CrCoNiFe HEA prepared by selective laser melting (SLM) have been studied. The results show that SLM-processed CrCoNiFe HEAs have a uniform microstructure and excellent tensile properties.
- The effect of cooling rate on the microstructure and mechanical properties of CrCoNiFe HEA has been investigated. The results show that a slower cooling rate can lead to a finer microstructure and improved mechanical properties.
- CrCoNiFe HEA has been explored as a promising material for hydrogen storage applications. The results show that CrCoNiFe
  HEA can store a significant amount of hydrogen and has good cycling stability.
- CrCoNiFe HEA has been investigated as a biocompatible material for biomedical applications. The results show that CrCoNiFe HEA is biocompatible and has potential applications in implants and other biomedical devices.

Overall, the recent academic papers on the CrCoNiFe system show that this material has a wide range of potential applications, including hydrogen storage and biomedical devices. Further research is needed to fully understand the properties and potential of CrCoNiFe HEAs.



Summarize this: High-entropy alloys (HEAs) are a popular research topic for materials scientists and engineers. Traditional steels have only one principal element, but HEAs have multiple, leading to high configuration entropy and a simple crystal structure [1]. Instead of one principal property, HEAs allow for multi-component systems that exhibit multiple desirable material properties. Strengthening mechanisms such as transformation-induced plasticity (TRIP) or twinning-induced plasticity (TWIP) alter the crystal structure of alloys to achieve desirable material properties, namely a combination of strength and ductility that is not found in traditional alloys. TRIP and TWIP mechanisms originated from steels and have been adopted into other systems since they are thought to be useful for many applications including the automotive industry because of their high energy absorption capacity and their ability to improve safety while reducing weight, chemical processing because of their corrosion resistant qualities, or aerospace because of their strength to weight ratio. Research on the fundamental mechanisms of these deformations aims to determine how they result in alloys [2,3]. Advancements in computational materials science aid in the development of accurate models for predicting phase diagrams for higher-order systems [4]. Sophisticated modeling and machine learning play a crucial role in predicting the behavior of systems with multiple principal elements.

The ternary CrCoNi system primarily has a face-centered cubic (FCC) crystal structure and has been extensively studied because of its unique mechanical properties, which exhibit higher strength and ductility than quaternary or quinary alloys made from this system [2]. Specifically, the well studied Cantor alloy has a much lower tensile strength, 491 MPa, compared to a tensile strength of 1 GPa for the ternary CrCoNi system [15]. This invalidates the idea that higher configurational entropy always leads to a better crystal structure and improved mechanical properties. Alloys containing 16 and 20 components in equal proportions have been studied, but have been found to be multiphase and brittle [5]. The well researched Cantor Alloy is based on this ternary system as well. Current research into quaternary or quinary alloys based on the CrCoNi system has focused on both equiatomic element concentrations as well as different compositions. Even small changes in elemental concentrations can have dramatic impacts on the microstructure and therefore the mechanical properties of alloys, but experiments take a long time to perform and are costly; therefore, modeling phase diagrams of higher-order systems is increasingly necessary to choose element concentrations with more potential before experimental verification.

## Literature Review:

Each element in an alloy system contributes to the mechanical properties and microstructure as well as the cost of manufacturing of the system, so additional elements added to a system must be chosen carefully. Cr is beneficial for corrosion resistance and Fe is cheap to manufacture, but both can cause the alloy to be brittle. Co has high hardness, but is expensive while Ni is a stable FCC element, so every element in the CrCoNiFe system benefits the mechanical properties of the system in a way, but the interaction of the elements must be examined carefully to determine the best concentration of each to enhance the strength and ductility of the alloy, without sacrificing either property, as well as improving other mechanical properties [4].

Niu et al. [6] in a study of the CrCoNiFe alloy found that in near-equal atomic concentrations certain elements of the system had the most significant influence on important mechanical properties, Cr on enthalpy of mixing and the ratio of bulk modulus to shear modulus, Co on lattice parameter and shear modulus, and Fe on bulk modulus.

Non-equal molar HEA systems based on the CrCoNi alloy have been found to possess good mechanical properties as well [4]. Mechanical modeling using computational materials design like CALPHAD allow for higher design diversity and preliminary testing of various elemental concentrations, accelerating the discovery of acceptable non-equimolar HEA systems. Feng et al. [4] found that a stable solid solution phase in a CrCoNiFe system can be created when the contents of Cr, Ni, and Fe are separately increased and studied for trends. This early acceptance of high design diversity

made possible by materials modeling showed the implications of changing elemental concentrations on crystal structures and properties of alloys. It was also found that both the enthalpy and entropy of mixing are important in determining the phase stability of an alloy, which further reiterates the findings from Otto et al. [7]. In this study, it was found that a large mixing entropy has more of an effect on phase stability than enthalpy. This helps to explain the low maximum Cr concentration in the solid solution island of the CrCoNiFe system found in this study, at only 25%. The maximum contents of the other elements of the solid solution island, Co, Ni and Fe could range up to 40%. This is in contrast to the Niu study which found that Cr concentration could be more influential on phase stability.

The importance of Cr concentration and manufacturing processes is further explored by Niu et al. [8] which looks into the importance of magnetic frustration of Cr in equiatomic CrCoNiFe solid solutions. It was found that ordering Cr eliminates magnetic frustration and in return reduces free energy in the system.

Further research into chemical ordering in the CrCoNiFe system by Brif et al. [9] using electron microscopy found that Cr was uniformly distributed throughout the alloy, but research into atomic ordering in the CrCoNiFe system by Lucas et al. [10] using x-ray and neutron diffraction found no long range chemical order in the alloy.

Work on adding additional micro-alloyed elements to the CrCoNiFe system has been found successful by teams such as Feng et al. [11]. The micro-alloyed elements could dissolve in small percentages in the system. Annealing the CrCoNiFe system alone was found to make stacking faults and twins occur in the matrix, while the addition of Al and Ti to the system lowered its stacking fault energy and promoted the formation of twins and stacking faults, respectively. This lower stacking fault energy experienced by the CrCoNiFe system micro-alloyed with other elements promotes higher strength and ductility in the alloy.

Salishchev et al. found that the annealing process did not affect the phase composition of the alloys in their study, including CrCoNiFe, CrCoNiFeMn, CrCoNiFeV, and CrCoNiFeMnV. Both CrCoNiFeMn were found to have a single phase FCC solid solution structure, while CrCoNiFeV and CrCoNiFeMnV had only FCC second-phase particles, due to the poor compatibility of V with the other alloying elements. The solid solution alloys are ductile and soft, while the CrCoNiFeV and CrCoNiFeMnV were strong, but brittle. Optimizing the fraction of FCC and  $\alpha$  phases from CrCoNiFeV and CrCoNiFeMnV systems are thought to result in an alloy with a desirable combination of strength and ductility.

Research into a similar alloy, FeMnNiCoCr, by Deng et al. [13] found that twinning only occurred under cryogenic conditions. The deformation substructure of the alloys studied were found to be strongly grain orientation dependent. A quaternary FeMnCoCr system was also part of the study and a non-equiatomic alloy, Fe40Mn40Co10Cr10, was found to be a single phase, homogenous FCC solid solution, whereas the equiatomic alloy was not

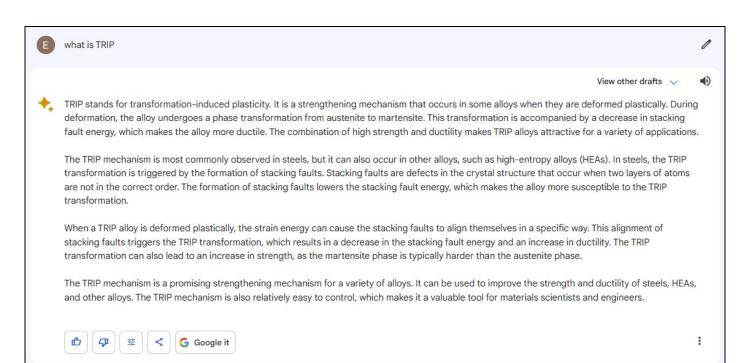
Sure, here is a summary of the text you provided:

- High-entropy alloys (HEAs) are a new class of materials that have been gaining popularity in recent years.
- · HEAs are made up of multiple elements, which leads to a high configuration entropy and a simple crystal structure.
- · This combination of properties makes HEAs very promising for a wide range of applications.
- . The CrCoNiFe system is one of the most well-studied HEA systems.
- · This system has been shown to have excellent mechanical properties, including high strength and ductility.
- · However, the addition of other elements to the CrCoNiFe system can also improve its properties.
- · For example, the addition of Al or Ti can lower the stacking fault energy of the alloy, which can lead to higher strength and ductility.
- · HEAs are still a relatively new class of materials, and there is still much research to be done.
- · However, the potential of HEAs is very promising, and they are likely to play an increasingly important role in future materials applications.

Here are some of the key points from the text:

- · HEAs are made up of multiple elements, which leads to a high configuration entropy and a simple crystal structure.
- · This combination of properties makes HEAs very promising for a wide range of applications.
- · The CrCoNiFe system is one of the most well-studied HEA systems.
- · This system has been shown to have excellent mechanical properties, including high strength and ductility.
- . The addition of other elements to the CrCoNiFe system can also improve its properties.
- · For example, the addition of AI or Ti can lower the stacking fault energy of the alloy, which can lead to higher strength and ductility.
- · HEAs are still a relatively new class of materials, and there is still much research to be done.
- · However, the potential of HEAs is very promising, and they are likely to play an increasingly important role in future materials applications.

I hope this summary is helpful!



**Appendix C:** The introduction and literature review produced from the case study.

Fundamental mechanisms of the CrCoNiFe high entropy alloy system Introduction:

High-entropy alloys (HEAs) are a popular research topic for material scientists and engineers. Traditional steels have only one principal element, whereas HEAs have multiple elements of high concentration, leading to high configuration entropy and a simple crystal structure [1]. Instead of one principal property, HEAs allow for multicomponent systems that exhibit multiple desirable material properties [2]. Strengthening mechanisms such as transformation-induced plasticity (TRIP) or twinning-induced plasticity (TWIP) alter the crystal structure of alloys to achieve desirable material properties, namely, a combination of strength and ductility that is not found in traditional alloys [3]. TRIP and TWIP mechanisms originate from steels and have been adopted into other systems because they are thought to be useful for many applications, including the automotive industry because of their high energy absorption capacity and their ability to improve safety while reducing weight, chemical processing because of their corrosion resistance qualities, or aerospace because of their strength-to-weight ratio [4,5]. Research on the fundamental mechanisms of these deformations is aimed at determining how they result in alloys [6,7]. Advancements in computational materials science have aided in the development of accurate models for predicting phase diagrams for higher-order systems [8]. Sophisticated modeling and machine learning play crucial roles in predicting the behavior of systems with multiple principal elements [9].

The ternary CrCoNi system primarily has a face-centered cubic (FCC) crystal structure and has been extensively studied because of its unique mechanical properties, exhibiting higher strength and ductility than quaternary or quinary alloys made from this system [6,10,11].

Specifically, the well-studied Cantor alloy has a much lower tensile strength (491 MPa) than the

ternary CrCoNi system tensile strength of 1 GPa [12,13]. This invalidates the idea that higher configurational entropy always leads to a better crystal structure and improved mechanical properties. Alloys containing 16 and 20 components in equal proportions have been studied; however, they are multiphase and brittle [14]. The well researched Cantor Alloy is based on this ternary system as well [12,15,16]. Current research on quaternary or quinary alloys based on the CrCoNi system has focused on both equiatomic element concentrations and different compositions [10,17]. Even small changes in elemental concentrations can have dramatic impacts on the microstructure and, therefore, the mechanical properties of alloys, but experiments take a long time to perform and are costly; therefore, modeling phase diagrams of higher-order systems is increasingly necessary to choose element concentrations with more potential before experimental verification [18,19].

To create an HEA based on the CrCoNi system, which has shown great promise for outstanding material properties, there must be sufficient deformation twinning [10, 20, 21]. With the help of phase-diagram modeling for high-order systems, the correct elemental concentration that promotes ideal mechanical properties can be achieved.

## Literature Review:

Each element in an alloy system contributes to its mechanical properties and microstructure, as well as the cost of manufacturing the system; therefore additional elements added to a system must be chosen carefully. Cr is beneficial for corrosion resistance and Fe is cheap to manufacture, but both can cause the alloy to become brittle. Co has a high hardness, but is expensive, while Ni is a stable FCC element, so every element in the CrCoNiFe system benefits the mechanical properties of the system in a way, but the interaction of the elements

must be examined carefully to determine the best concentration of each element to enhance the strength and ductility of the alloy, without sacrificing either property, as well as improving other mechanical properties [8].

Niu et al. [22] in a study of the CrCoNiFe alloy found that at near-equal atomic concentrations, certain elements of the system had the most significant influence on important mechanical properties: Cr on the enthalpy of mixing and the ratio of bulk modulus to shear modulus, Co on the lattice parameter and shear modulus, and Fe on the bulk modulus.

Non-equal-molar HEA systems based on CrCoNi alloys have also been found to exhibit good mechanical properties [8]. Mechanical modeling using computational materials design, such as CALPHAD, allows for higher design diversity and preliminary testing of various elemental concentrations, accelerating the discovery of acceptable non-equimolar HEA systems. Feng et al. [8] found that a stable solid solution phase in a CrCoNiFe system can be created when the contents of Cr, Ni, and Fe are separately increased and studied for trends. This early acceptance of the high design diversity made possible by material modeling showed the implications of changing elemental concentrations on the crystal structures and properties of alloys. It was also found that both the enthalpy and entropy of mixing are important in determining the phase stability of an alloy, which further reiterates the findings of Otto et al. [23]. In this study, it was found that a large mixing entropy has a greater effect on phase stability than enthalpy. This explains the low maximum Cr concentration of only 25% in the solid solution island of the CrCoNiFe system found in this study. The maximum contents of the other elements in the solid solution island, Co, Ni, and Fe, could range up to 40%. This is in contrast to the Niu study, which found that the Cr concentration could be more influential on phase stability.

The importance of Cr concentration and manufacturing processes was further explored by Niu et al. [24], who examined into the importance of the magnetic frustration of Cr in equiatomic CrCoNiFe solid solutions. It was found that ordering Cr eliminated magnetic frustration and reduced the free energy in the system.

Further research on chemical ordering in the CrCoNiFe system by Brif et al. [25] using electron microscopy revealed that Cr was uniformly distributed throughout the alloy, but research on atomic ordering in the CrCoNiFe system by Lucas et al. [26] using X-ray and neutron diffraction found no long-range chemical order in the alloy.

The addition of micro-alloyed elements to the CrCoNiFe system has been successfully achieved by teams such as Feng et al. [27]. Micro-alloyed elements can dissolve in small percentages in the system. Annealing the CrCoNiFe system alone was found to cause stacking faults and twins in the matrix [28], whereas the addition of Al and Ti to the system lowered its stacking fault energy and promoted the formation of twins and stacking faults, respectively. The lower stacking fault energy experienced by the CrCoNiFe system microalloyed with other elements promotes higher strength and ductility in the alloy.

Salishchev et al. [15] found that the annealing process did not affect the phase composition of alloys in their study, including CrCoNiFe, CrCoNiFeMn, CrCoNiFeV, and CrCoNiFeMnV. Both CrCoNiFe and CrCoNiFeMn were found to have a single-phase FCC solid solution structure, whereas CrCoNiFeV and CrCoNiFeMnV had only FCC second-phase particles due to the poor compatibility of V with the other alloying elements. The solid solution alloys were ductile and soft, while CrCoNiFeV and CrCoNiFeMnV were strong, but brittle. Optimizing the fraction of FCC and  $\alpha$  phases from CrCoNiFeV and CrCoNiFeMnV systems are thought to result in an alloy with a desirable combination of strength and ductility.

Research on a similar alloy, FeMnNiCoCr, by Deng et al. [29], found that twinning only occurred under cryogenic conditions [30]. The deformation substructure of the studied alloys was found to be strongly dependent on the grain orientation. A quaternary FeMnCoCr system was also part of the study, and a non equiatomic alloy, Fe<sub>40</sub>Mn<sub>40</sub>Co<sub>10</sub>Cr<sub>10</sub>, was found to be a single-phase, homogenous FCC solid solution, whereas the equiatomic alloy was not. Borja also found that the strength of the CrCoNiFe alloy increased at the liquid-helium temperature without sacrificing ductility [31].

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