Material Science and Artificial Intelligence: Insights from Professor Demircan Canadinç

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***Abstract*— In this interview, Professor Demircan Canadinc of Koç University explains his work at the intersection of material science and artificial intelligence (AI). Professor Canadinc has concentrated on the deformation of metallic substances as his area of expertise in the area of mechanics of materials. His current research, in collaboration with important institutions like Los Alamos National Laboratory, transforms the design of high-strength, smart shape memory alloys, and biomedically compatible metallic materials. His work addresses the challenges of creating alloys with a Young's modulus akin to human bone for orthopedic implants. Professor Canadinc uses AI to optimize the alloy composition with exceptional speed and efficiency which is a breakthrough that significantly improves upon the traditional, decades-long trial-and-error cycle in material design. This interview with Professor Canadinc explores the utilization of state-of-the-art techniques such as SEM and XPES housed in KUTTAM (Koç University Research Center for Translational Medicine) laboratory for the characterization of newly minted alloys. Professor Canadinc also sheds light on the broader usage of AI in materials science and his anticipation for the future applications of AI in the field.**

Keywords—artificial intelligence in alloy design, deformation of metallic materials, material science, mechanical engineering, shape memory alloys

I. Introduction

Professor Demircan Canadinç is a material scientist and a professor at Koç University in the Department of Mechanical Engineering. By training, he is a mechanical engineer, as he has acquired all his degrees in mechanical engineering. In his research, his focus lies in the mechanics of materials.

He specializes in the deformation of metallic materials, specifically high-strength materials - shape memory alloys that are a class of the so-called smart materials - and biomedical metallic materials, such as implant materials. Professor Canadinç focuses on the design of their microstructures, compositions, and response to the mechanical loading under both monotonic and cyclic loading that is the fatigue behavior or, in other words, long-term behavior. Lately, he has been designing alloys using artificial intelligence.

> *"I took an introductory materials science course as an undergraduate student. After that, I was hooked!"*

His journey with material science started back when he was an undergraduate student. The material response and metals attracted his attention. For that reason, he wanted to get involved in the solution of material problems, especially those concerning metals.

II. Current Research

Professor Canadinç is involved in a few research areas that are important in many applications, including biomedical applications. In collaboration with Los Alamos National Laboratory in the United States, his research team designed new metallic materials using artificial intelligence that would exhibit high strength at elevated temperatures while also maintaining formability at low temperatures. In collaboration with his graduate students, he also addressed the problem of designing a biocompatible metallic implant material for orthopedic implants, ensuring that the mechanical biocompatibility is also satisfied. As bone has a very low elastic modulus and metals have much higher values than that, they wanted to design a metallic material that is both strong, formable into the desired shape, and exhibits Young's modulus, a measure of elasticity commonly used in material science, that is as close as possible to that of the bone. They used artificial intelligence to come up with the chemical composition that would give the desired result (Process summarized in Figure 1). We had an opportunity to ask a few questions about the details of his research during our interview.

A. How is Artificial Intelligence Used in Your Research?

"Firstly, we run different machine learning algorithms with different mathematical linearities that go over data we collected through experiments and literature on similar materials - data reported on existing and known materials. Then we train the algorithms, compare their performance, and pick the best one upon testing. The training is done on 80% of the data, so the algorithms never see the other 20% of the data. Once we train them, meaning that once the algorithm learns the unseen relationships we cannot see with the human eye, it creates mathematical functions. Once the functions are done,

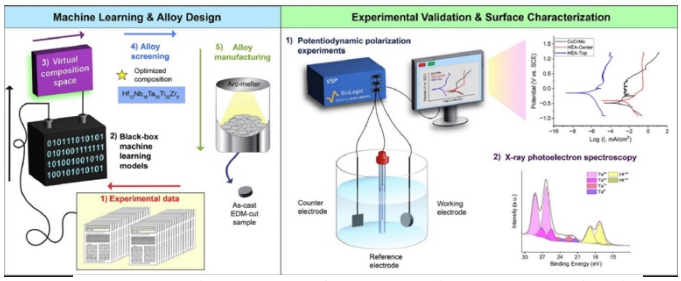

Figure 1 The Process of creating alloys using Artificial Intelligence. [1]

Interview Conducted: 02.04.2024 | Manuscript Reviewed: 12.04.2024 | DOI: 10.5281/zenodo.10963182

we test those functions on the other 20% that algorithms have never seen before and pick the best-performing algorithm. Finally, we make predictions with that algorithm to discover new alloys."

"After the new alloys are discovered, the researchers choose some of them to be manufactured and tested in real life. Depending on the level of precision various companies can manufacture the alloys. Typically, for high-precision manufacturing, there are special companies that focus on manufacturing exactly what the customers want. For some of the articles, Professor and his group collaborated with the TUŞAS Engines Industry, a Turkish company specializing in jet engines, which can produce materials with high precision. However, if such collaborations are not available, there are companies outside from which they can order the material. Therefore, when designing a material numerically, researchers ask for a given composition and then either order the material from outside vendors or have collaborators produce it for them. After that, the process of characterizing the material begins."

B. *How are the Alloys Created by Artificial Intelligence Characterized?*

"For characterization purposes, we use the facilities at KUTTAM (Koç University Research Center for Translational Medicine). In my lab, there are simple setups for biocompatibility testing of biomedical materials. With the help of these setups, we emerge the samples in fluids that simulate the body environment, such as artificial saliva and artificial blood. We then check if the designed material satisfies the basic biocompatibility criteria. If it passes, we then proceed to the next level. For the characterization of those fluids and the sample surfaces, we use KUTTAM facilities. We use equipment such as Scanning Electron Microscopy (SEM) (Figure 2), X-ray photoelectron Spectroscopy (XPES) for surface oxidation analysis, X-ray diffraction for examining the material phases and texture, and Field Emission Electron Microscopy (FEACM). Additionally, for compatibility analysis to determine the amount of ions in the simulation fluids, we use Inductively Coupled Plasma Mass Spectrometry (ICPMS). These are different techniques that we use and all of them are available in KUTTAM, which is why we carry out our research mostly at Koç University."

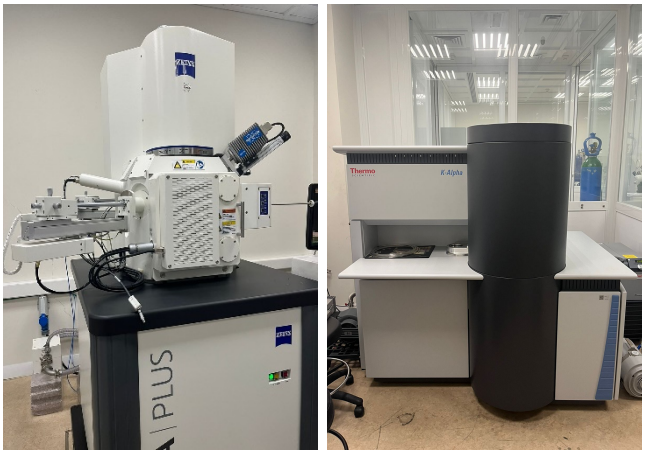

Figure 2: Scanning Electron Microscope (SEM) and X-Ray Photoelectron Spectroscopy in the KUTTAM laboratory at Koç University

C. *How do You Decide Which Materials to Focus on Given the Abundance of Options?*

"As engineers, when designing a material, we always need to make decisions. For instance, with implant materials or biocompatible alloys we need to make sure that all the constituent elements of the alloy are also biocompatible by themselves. For that reason, we have Titanium, Tantalum, and Zirconium in those alloys. We do not include Aluminum, as it can cause Alzheimer's or other disorders. With that being said, the selection is not always AI-based or random, there are some engineering decisions in the first place."

"Element-wise, we only use metals listed in the periodic table that are naturally occurring on Earth. Usually, these metals are found in the form of compounds, so we need to separate them and that is what makes the rare metals expensive. We usually use metal powder in order to create new alloys. In terms of powder, there is a process called the atomization process, which allows the making of powders of any metal. However, this process is very specialized, and atomizing is already expensive, and rare metals like titanium, tantalum, or polonium make the metal powders even more expensive."

III. Limitations That Material Science is Facing

In our world governed by the laws of capitalism and supply and demand, many less profitable industries are experiencing difficulties. Some branches of scientific research are unfortunately considered to be less useful by society. Hence many researchers are facing various problems during their careers. We asked Prof. Demircan to tell us about some limitations he is facing throughout his research.

"Limitations in my field are mostly related to finances. Characterization equipment is very expensive, which is why we use a centralized laboratory here. Additionally, the cost of metal powders is rising as they are getting rare, and high-performance metals and alloys usually require the utility of some of those rare metals. Experimentation costs are high as well. Moreover, you need to have people willing to do research in the metallurgy field. These days, interest is mostly in computer science and while combining those two fields, as I do, can help, human interest remains an issue. When it comes to implant materials research, certain regulations are coming from such organizations as FDA in the United States, or Sağlık Bakanlığı (Ministry of Health) here in Turkey. Certain regulations need to be followed before testing on humans can proceed. Of course, they are actually needed, so I wouldn't say it is a barrier, but it makes things go slow."

IV. The Future of Artificial Intelligence In Materials Science

Nowadays, the rapid advancements in Artificial Intelligence (AI) create a lot of change in many sectors and industries, from autonomous driving, and simple speech recognition to even manufacturing. Research and academia are no exception and neither is Material Science. AI has been increasingly utilized in material science to accelerate research, enhance understanding, and discover novel materials with desired properties.

A. *What is Your Opinion on the Current Use of AI in Materials Science?*

"Traditionally, using conventional metallurgic approaches to design a new class material, make trial and error, come up with a usable design and prove that it works, it takes between 10 to 30 years. However, when AI and existing data are used, it takes only around 6 to 12 months. Other researchers showed that the cost decreases by 90-95% due to the elimination of trial and error. Imagine a composition space as big as this office room, but target compositions are in the place of this bottle on the table. AI is directing you towards this bottle instead of going through all of the space experimentally. Of course, when the material is designed and manufactured, we need to conduct the experiments to validate our predictions, but we do not experiment with all possible compositions and that saves a lot of time."

B. *What about the Future of Materials Science? Does AI Have A Place in It?*

"The future is as follows, but I am not sure when it is going to come. There will be problems and solutions to these problems will be detected by artificial intelligence. Given the duty, AI will decide itself on the solution method, come up with a prediction, make the alloy, test it, and then give us the solution. I think it will be implemented in the manufacturing processes in all the disciplines. But how long it will take - I don't know. However, at some point, it might change. This is the future aim, so how much of it will be accomplished or how much of it will be allowed by the society remains to be seen."

> *"People like us will be mostly eliminated or maybe just directing the processes. But right now, it needs engineering decisions made by engineers."*

V. Personal Advice from Professor Canadinç

Falling in love with science, regardless of the type, is quite easy but deciding to become a scientist and to spend your life as a researcher, can be scary and overwhelming for some people, especially young and indecisive college students. Knowing that our audience is probably people who are interested in research, we decided to ask our interviewee a question that aims to give college students some direction.

A. *What advice would you give to someone studying material science in terms of selecting areas of focus, considering the interdisciplinary nature of current problems?*

"Well, this advice is valid for all the disciplines, but in the case of material science, it is an old field, not a new one. I would recommend learning the basics very well and then expanding the knowledge not only in the area of interest but also equipping themselves with additional tools such as machine learning, chemical engineering, chemistry, medicine, or biology. That would definitely help with the interdisciplinary problems. I would recommend not being an expert on one thing only, but also expanding the knowledge in different directions, because many problems these days are interdisciplinary. I would try to focus on the intersection points of different disciplines with material science and then equip myself with the necessary tools depending on my interest. That is the advice that I would like to give."

Many people consider research to be one of those industries that no one knows the details about because it is not as popularized as more common industries. We always hear the success stories but never the difficulties that the researchers are facing. The industry often seems to be impersonal. This can create a lot of uncertainty in the minds of aspiring scientists. To try and balance it out, we asked Professor Canadinç to tell us about the difficulties he personally faces as a material scientist in Turkiye.

"Everybody faces similar challenges, but there are also some personal ones. Some of these problems are related to Turkiye because the industry-academia relationship is not where it should be. This limits your ability to expand your horizons and reach out to the ones who can actually use your research outputs. Additionally, metallurgy is an old field - more than a century old - with its roots tracing back to the Stone Age, if we look at it practically. While it means that there is a lot of knowledge, it also means that there are many people in this field and the problems are not considered exciting anymore. This makes the research funding limited, as opposed to AI research in computer science, for instance. Carrying out research without proper funding becomes difficult."

VI. Conclusion

In this interview, Professor Canadinç gave us a lot of insights about his research areas and the way the industry works in general. He touched upon the topics of the importance of Artificial Intelligence, and the potential future of material science. For our aspiring scientists, he also shared some advice and potential challenges that may be faced during the journey of becoming a researcher.

Acknowledgments

We would like to express our sincere gratitude to our first guest professor who is featured in this journal, Professor Demircan Canadinç, for accepting our invitation, letting us conduct the interview, and showing us around the KUTTAM laboratory at Koç University. We are also thankful to the staff at KUTTAM for telling us about the various equipment and letting us take some pictures while we were there. We would like to say that this was an amazing experience for us and we learned a lot of things throughout this interview.

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