ME – MTech(Res) Thesis Defence

Inverse Material Design using Deep Convolutional Neural Networks (CNN) and Ontology

Mr. Anand Kumar Patel, MTech(Res) Student, Department of Mechanical Engineering, IISc Bengaluru

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ABSTRACT

Materials design is the process of tailoring materials with specific properties and performance characteristics to meet the particular needs of an application. It involves going back on the process-structure-property (PSP) relation from properties to manufacturing processes. Consequently, much research has dived into PSP relation modeling, and recently, data-driven methodologies for modeling PSP relations are becoming a way of research in the field. However, most of the efforts investigate only the structure-property relation, leaving the other part relatively unexplored. Moreover, they tend to focus only on specific material systems and lack the consideration for microstructural metadata (The peripheral and metallurgical data related to the microstructure such as material composition, magnification, primary microconstituents and their phase volumes, grain size and morphology, etc.); These limitations are perhaps in part due to the absence of a standards format or protocol for collecting, storing, and sharing the PSP relationship datasets. Also, much of the knowledge in the field of materials design and materials science is primarily empirical and experiential. Consequently, capturing this prior knowledge in a structured, human-readable, and computable format is necessary. The handling of the sequential data regarding the manufacturing processes undergone by materials is yet another open area of research.

In this work, we develop a scalable convolutional neural network (CNN) based approach for modeling the inverse process-structure relation using Ultrahigh carbon steel and Ni-Co alloy materials datasets. Here, the scalability of the models was achieved by implementing multi-input multi-output CNN models on various learnable relations. Learnable relations included a variety of direct approaches and a feature augmentation-based approach. The assortment of models concluded that the direct approach models having microstructure and its metadata both as input produced the best results for predicting the process parameters. Thus, formalizing the intuitive importance of microstructure metadata. In addition, typical problems with the PSP relationship datasets were identified, and potential solutions such as data and test-time augmentation techniques and an ontology-based standardization were suggested and evaluated.

To implement the above-mentioned solution and capture some of the essential knowledge in the materials design field in a structured and computable format, an application ontology called PSPOnto was developed. The devised ontology could readily handle data regarding the complete manufacturing history of a material, along with its microstructure and properties, in a generic way. Provisions for capturing the details of microstructure preparation methods and material property measurement procedures were also made. PSPOnto was designed to preserve and exploit the capabilities of an ontology in handling the many-to-many relations among the entities stored in it. Consequently, the novel structure of the ontology enabled a conventional SPARQL query engine to search for the materials with specified property requirements and the associated manufacturing process sequences without any ab-initio manufacturing process sequences being input into the knowledge base. Thus, PSPOnto is regarded as laying the foundation for the knowledge-based establishment of PSP relations and materials design. The proposed ontology was then validated for its efficacy by creating a knowledge base on it using a Ni-Co alloy dataset and querying it using the SPARQL query language. The exhaustive enumeration of the manufacturing processes, corresponding process parameters, and the compilation of reference articles used in its creation serve as an independent resource for other researchers working on PSP relations and accelerated materials design.

Area of Research Topic: Data-driven modeling of Process-Structure-Property relationships

Field of Investigation: Materials Informatics

ABOUT THE SPEAKER

Mr. Anand kumar Patel is an M. Tech (Research) student in the Department of Mechanical Engineering, IISc, Bengaluru. He completed his B. Tech from Birla Vishvakarma Mahavidyalaya Eng. College, Vallabh Vidyanagar, in 2021. Subsequently, he has been working with Prof. B. Gurumoorthy in the Product Lifecycle Management (PLM) lab. His research interests are broadly in materials design and data-driven modeling of Process-Structure-Property relationships.