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THE POTENTIAL UTILITY OF MATERIALS INFORMATICS IN DEVELOPING NON-CONVENTIONAL MATERIALS

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ABSTRACT

Materials informatics is widely acknowledged as a means of accelerating the rate of new materials discovery and material development. Such an approach will require widespread use of data driven methodologies and it is anticipated that downstream stakeholders, particularly industry, will be heavily involved in providing the required resources. This paper will propose workflows that illustrate how data driven methods could reasonably be applied to the processing-structure-properties relationships of locally sourced non-conventional materials. It is anticipated that simple material tests and imaging techniques will provide sufficient digital information for data driven approaches at relatively low cost. This utility will be illustrated using the example of bamboo and the levels of structure observable using widely available digital phone cameras. Finally, the possible role of the NOCMAT community in facilitating materials informatics will be considered.

Keywords: Non-Conventional, Materials, Informatics.

INTRODUCTION

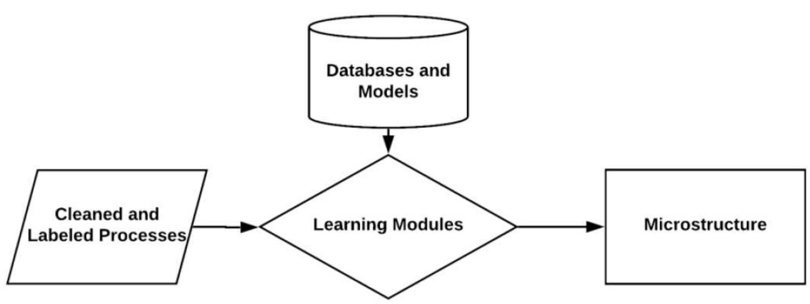
New materials discovery and development has traditionally been a subject dominated by experimental approaches with relatively long development cycles of 20 years or more. The Materials Genome Initiative in the USA is a multidisciplinary, collaborative approach focused on shortening development cycles for materials by promoting major roles for computational modeling and simulation techniques of different types. Unfortunately, physics based modeling approaches – whether density functional theory for electron structure [1], thermodynamic modeling of phase stability [2], phase field modeling of microstructure or finite element analysis at the macroscopic scale – are often challenged by structural complexity. The multiple levels of structure in many materials have further limited the wider contributions of physics based modeling. Data driven modeling approaches are more suited to solving complex problems. Materials informatics [3] is a more recent application of data modeling approaches and while it does involve the core requirements of data capture, database management and data analysis it is also a basis for information based learning [4], through which new materials science could be discovered. Implicit in the practice of materials informatics is the participation of a committed community that has agreed to devote resources to the collection of trusted data and its consequent aggregation into curated databases that can be made available to those working in the community. This will take significant investment, especially if the data collection is expensive, requiring sophisticated, specialized equipment.

This paper will describe the potential of materials informatics to address the issues that contribute to the variability in the properties of locally sourced, non-conventional materials and also speculate on how such an approach might be implemented with suitable work flows. The specific example of full-culm bamboo will be considered. Finally, the expected challenges and potential benefits will be discussed.

MATERIALS INFORMATICS AND ITS APPLICATION TO NON-CONVENTIONAL MATERIALS

Briefly, materials informatics [3] is the application of information engineering to materials science and engineering. Data driven approaches such as machine learning and artificial intelligence, discover new knowledge through the generation, management and analysis of data. These techniques are able to efficiently deal with degrees of complexity that challenge physics based methods traditionally used in materials science and engineering.

The widely accepted materials science and engineering paradigm has within it three sources of data. Processing data derived from all the materials refining and manufacturing processes, materials structure data from all the levels of structure and finally all the different types of material property data. Data driven methods are used to predict relationships between designated inputs and outputs and thus it is necessary to decide which of the three types of data will be inputs and which will be outputs. Directly inferring relationships between materials processing and material properties is not desirable because it implicitly denies the central role of materials structure in developing new materials. It is therefore necessary to develop data driven models for both processing-structure and structure-properties relationships as shown in Fig.1. It is also necessary to assemble suitable information into accessible databases. Indeed, the availability of suitable data in appropriate formats will be of vital importance to the success of this type of research.



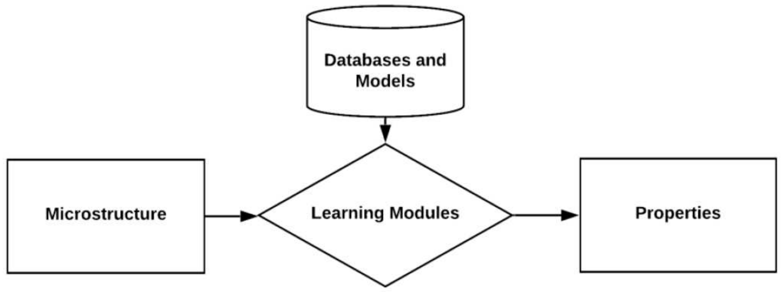


FIGURE 1: THE APPLICATION OF DATA DRIVEN METHODS TO THE MATERIALS PROCESSING-STRUCTURE-PROPERTIES PARADIGM.

In general, the databases needed for data driven materials discovery and development are not well developed across the materials processing-structure-property paradigm. Some traditional subjects such as basic crystallographic and thermodynamic information have been assembled into databases with some success while other topics suffer from a lack of coverage. The aggregation of data into searchable databases must accelerate if materials informatics it to fulfill its promise; several initiatives are being developed in this realm. In the US, for example, the National Institute of Standards and Technology (NIST) has taken a leading role in coordinating the necessary infrastructure and data resources in their Materials Genome Initiative [5], consistent with their traditional role in evaluation of data, data curation and data integration for materials. Specific materials data resources include the Materials Resource Registry [6], an inventory of materials databases, tools and repositories that can be accessed from anywhere in the world. In addition, the NIST Materials Data Repository [7] has the objective of improving the quality of materials data by establishing mechanisms for sharing data and best practices for management of materials databases.

Once databases of sufficient utility become available it will be necessary for materials science and engineering practitioners to become familiar with widely available data science techniques that could be used for establishing new processing-structure and structure-property relationships. At present even relatively simple methods such as principal component analysis, which correlates a set of recorded observations into a set of linearly uncorrelated outputs called principal components, is not well represented in materials science and engineering curricula at universities. More complex methods such as neural networks are capable of capturing non-linear relationships between each desired material output and the sum of all the material input observations [8]. The neural network "learns" by changing the weighting of the relationships between the input and output nodes called neurons as more data is added. While techniques such as neural networks have demonstrated great utility, they require proper model training and the user must have significant knowledge and understanding to correctly apply them.

At present, materials informatics has not been applied to non-conventional materials in any meaningful way. There are some databases that contain information on locally sourced materials such as wood. MatWeb [9], for example, contains property data for 306 different woods and wood based composites but such sources are rare and not sufficient to implement data analysis techniques for structure-property relationships. In particular there is relatively little archived information concerning the structure of non-conventional materials. This is somewhat inhibited by the wide range of important lengthscales in the structure of many non-conventional materials that, if they are to be fully quantified, would require characterization tools ranging from optical microscopes to transmission electron microscopes to micro tomography and x-ray diffraction. Many such tools are not easily accessed by practitioners working with non-conventional materials. Such data would also have to be compiled into standard formats that could be inputted into microstructure analysis kernels. These requirements raises real questions of social equity in materials informatics given that resources required for database development, curation and maintenance are, in theory, to come from downstream stakeholders

If data driven techniques are to be applied by the non-conventional materials community there is a need to come to agreement on their foreseen role, the nature of the information to be collected, data formats, accompanying metadata requirements and the organizations and institutions that would host such resources. Since non-conventional materials are locally sourced the processing-structure information should be collected in the field and so the required information must be constrained in ways that would make collection and submission of information feasible. Structure-property information is expected to be more limited but of higher fidelity if standard tests are used. Property information could also come from field tests if they were standardized but are more likely to come from laboratory testing. Fig.2 summarizes a proposed work flow by which materials processing-structure information collected in the field using a phone camera and information from laboratory tests could be combined into a materials informatics approach to non-conventional materials engineering. This will now be further explained in the context of bamboo.

THE EXAMPLE OF BAMBOO INFORMATICS

Bamboo, like wood, is derived from living tissue and therefore the levels of materials structure have evolved to function while the plant is alive and then degrade after the life cycle is complete. In contrast, for engineering applications, the plant is grown to a suitable maturity before harvesting, drying and treating. With the natural function of bamboo in mind, qualitative comparisons have been made between the levels of structure in bamboo and other natural materials and their biological function [10]. These levels of structure have been identified and imaged by a variety of techniques for bamboo [11-14]. The structure at some of these different scales is known to vary from species to species [15] and be sensitive to grow location and growth conditions. Once harvested, dried and treated, the properties of bamboo are dominated by fibers aligned with the axis of the culm and the fact that the culm is hollow. It is therefore reasonable to study the properties of bamboo in analogy with composites containing stiff aligned fibers. Hence, the axial properties, like elastic modulus Ec, are quantified using familiar concepts such as the rule of mixtures in Eq. 1.

$$E_c = (V_f E_f) + ((1-V_f)E_m) \tag{1}$$

Where Ef is the elastic modulus of the fiber, Em is the elastic modulus of the matrix and Vf is the volume fraction of the fibers. This basic relationship has been adapted to take into account the variation in fiber volume fraction through the culm wall [16-19].

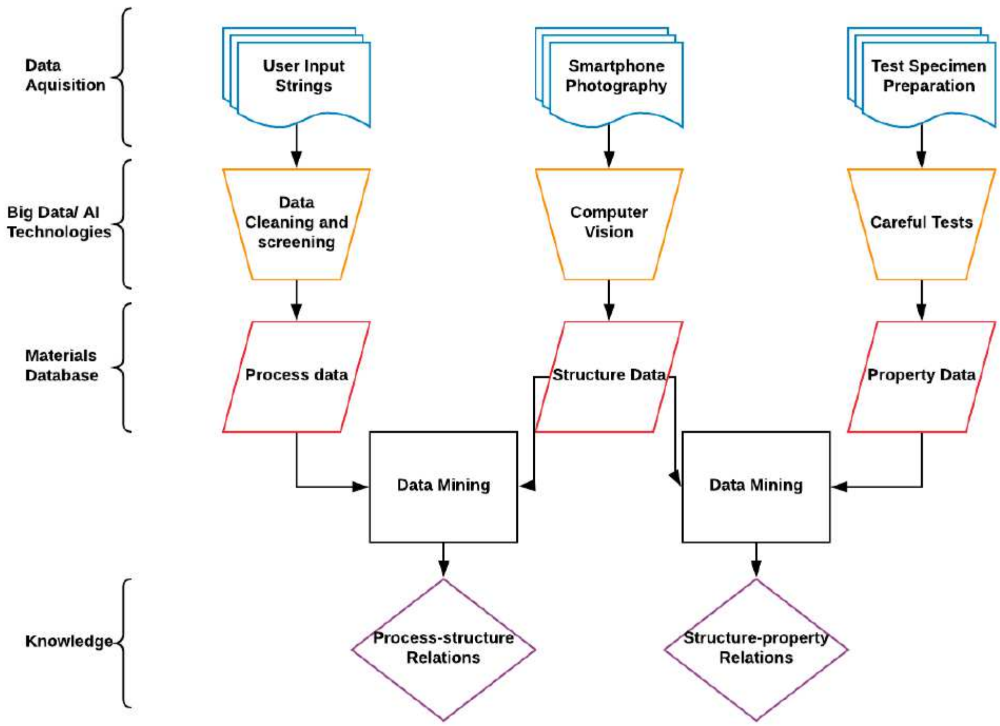


FIGURE 2: PROPOSED WORKFLOWS FOR PROCESSING-STRUCTURE AND STRUCTURE-PROPERTY RELATIONSHIP DETERMINATIONS FOR NON-CONVENTIONAL MATERIALS

Eq. 1 contains only one structural parameter, the volume fraction of the fibers and assumes two distinct and homogeneous phases. Examination of the structure at higher magnifications using electron microscopy and atomic force microscopy reveals a rich complexity that defies the notion of homogeneous reinforcing and matrix phases. While not representing all the levels of structure, Fig.3 shows a scanning electron micrograph that reveals the fibers are collected into fiber bundles that also contain hollow capillaries. The shape and internal structure of the fiber bundles varies from species to species and also through the thickness of the culm wall. Surrounding the fiber bundles is the parenchymal matrix made up of relatively large hollow cells.

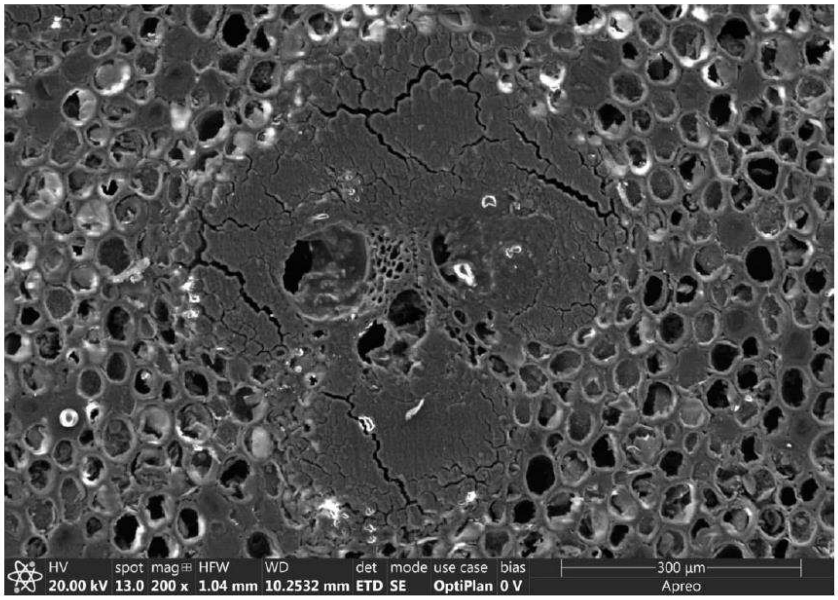


FIGURE 3: SEM MICROGRAPH OF A POLISHED SECTION OF BAMBOO

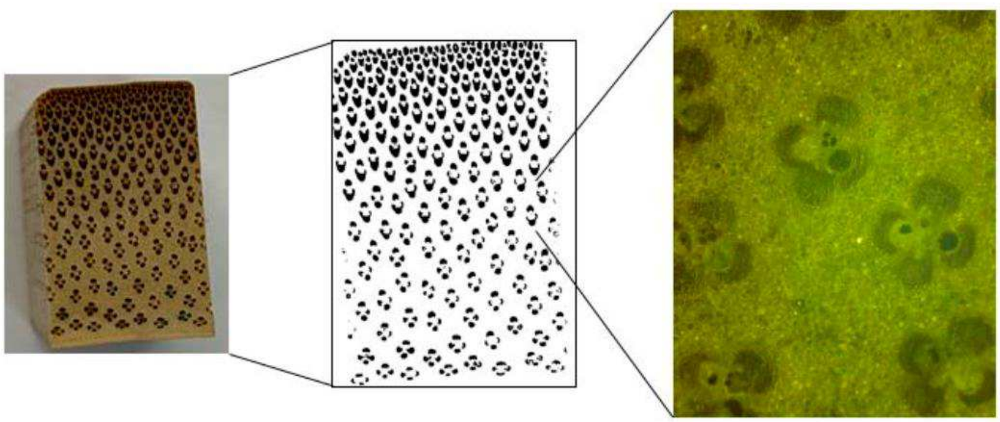


FIGURE 4: OPTICAL MICROGRAPH REPRESENTATIVE OF THAT TAKEN WITH A PHONE CAMERA AND THE CONSEQUENT PROCESSED IMAGE THAT ASSUMMES TWO PHASES. A HIGHER MAGNIFICATION OPTICAL MICROGRAPH OF THE BAMBOO STRUCTURE

If the rule of mixtures is a representative relationship, it is possible to make some interesting assumptions that would allow the structure of bamboo to be imaged and quantified using a simple phone camera suitable for use in the field. Fig. 4 shows such an optical image in which fiber bundles are distinctive due to their dark contrast. The accompanying processed image that assumes the material is two phases is also shown. The higher magnification optical micrograph shows that the vessels associated with the fiber bundles will also have the same dark contrast and thus be included in the measured fiber bundle area fraction. Thus it is clear that the practitioners working on bamboo will have to agree on how the contrast is to be interpreted during data processing by computer vision methods. While these assumptions do not take into account any variation in the internal structure of the fiber bundles, it does, under the constraints of the contrast conditions, allow the gradient in fiber volume fraction along the thickness of the culm wall to be estimated. It is thought that the variation in the gradient of fiber bundles volume fraction is responsible for much of the variation of axial properties. If this proves to be the case, one could envision that examination of the natural variation of the gradient of fiber bundles across the culm wall and the influence of species and growth locations and conditions would be able to explain the variation in axial properties of bamboo. Much more data will be needed if the application of data driven approaches are to develop a better understanding of the variability in the axial properties of bamboo.

The transverse properties of bamboo, on the other hand, are dominated by weak interfaces that commonly lead to splitting. In this circumstance, rule of mixtures for transverse loading is not expected to be particularly meaningful, especially when the variability in experimentally measured properties is large. Therefore, the correlation of the transverse properties of bamboo to structure observed using a simple phone camera will be more challenging. In particular, the transverse properties of bamboo appear to be dominated by the strength of the interfaces between the cell walls in the parenchyma [20] and cracking within the fiber bundles [21]. The phone camera might be able to determine if the transverse failure occurred through the fiber bundles or through the parenchyma cell walls but the interpretation will be more nuanced.

Although imaging of the volume fraction of fibers can be done in the field with a camera phone, this does not realize the database(s) required to generate, clean, store and maintain this information in a form that can be input into common data analytic tools. This must be done under the guidance of the NOCMAT community with an enduring commitment of its members to participate. It is important that the community agree on the standards used for capturing, transmitting, sharing and curating such information.

SUMMARY

Materials informatics is a data driven approach that has been proposed as an alternative means of discovering new materials and managing materials development. This is particularly attractive when the materials structure is complex with several levels that can influence desired properties. This complexity can lead to significant variability between experimental measurements on nominally the same material and confound physics based modeling approaches. While it is quite obvious that data driven approaches are proving their worth for complex problem solving in a variety of fields, they do require research communities to commit to developing standards and infrastructure for data acquisition, transmission, storage and sharing. In the case of materials informatics, there is also a need to divide the processing-structure-properties paradigm into processing-structure and structure-properties relationships to facilitate the application of data science techniques. These techniques could be as simple as principal component analysis or they might require more complicated models such as neural network and the attendant specialized knowledge. The infrastructure and standards for materials informatics have been slow to evolve since it was proposed over 10 years ago. However, recent developments such as the Materials Genome Initiative are beginning to gain influence in this respect.

The ability of materials informatics to address complexity is quite attractive in the case of natural, locally sourced non-conventional materials which are characterized by a continued lack of effective materials standards and the wide variability in properties. It is not very difficult to propose that materials information from simple field tests and observations could be collected at practically any location with a camera phone and shared with the community. This prospect does indeed play to the strengths of data driven approaches for materials development. However, the challenges associated with resources development and the collective commitment required to develop standards for data acquisition, transmission, storage and sharing should not to be underestimated. In the world of highly controlled materials the resources for database curation and management will probably come from the downstream stakeholders including multinational industries and governments. In the case of locally sourced non-conventional materials that serve relatively poor communities, the resource requirement raises significant issues of social equity. This manuscript has described how, in the example of full-culm bamboo, it may be possible to constrain the data acquisition to relatively inexpensive and widely available technologies that lower the barrier to the application of materials informatics to non-conventional materials. Since, this would be a collective endeavor it is critically important that the non-conventional materials community provide leadership in the development of standards and infrastructure so that participation would be broad and sustained with the benefits being widely shared.

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