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A method for reverse engineering of material microstructure for heterogeneous CAD

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ABSTRACT

Integration of material composition, microstructure, and mechanical properties with geometry information enables design and analysis of materials and products in a computer-aided design (CAD) environment. In this paper, we propose a method for the construction of material models from microstructure images, that can be integrated into a heterogeneous CAD representation. The method utilizes Radon and wavelet transforms to compute a surfacelet representation. A novel feature recognition method was developed to identify microstructure features, including embedded fibers and grain boundaries, from the surfacelet representation. The models and methods were demonstrated with examples of synthetic and engineered polymer nanocomposites, a metal alloy, and a medical dataset of human feet.

1. Introduction

The capability of deriving mechanical properties from the material and geometry information in computer-aided design (CAD) tools would greatly aid materials and component design. In heterogeneous CAD modeling, models of both part, geometry and material composition, are integrated. In existing methods, material composition is typically specified parametrically using volume fractions where continuous distributions of material compositions are modeled. This approach is only appropriate for macro-scale part models, where detailed microscopic structures are not considered. Furthermore, such material composition models only represent the designer's desires or specifications, but the physical behavior of the actual materials is not recognized. As such, the actual material composition may deviate from the specification due to the specifics of manufacturing processes, heat treatments, or other material limitations. For example, with some metal alloys, one constituent metal may dissolve in another, only up to a certain volume fraction, but may segregate at higher volume fractions, or form very different microstructures.

In order to support integration of microscopic material models into CAD models, at least two requirements must be met. First, extensive process–structure–property relationships must be captured and integrated with the geometric model in the CAD system. This will allow detailed compositions of actual materials to be captured. Second, it must be possible to generate material microstructure models at various size scales; hence, methods for multi-scale and multi-resolution modeling are needed.

In recognition of the need of microscopic materials modeling for heterogeneous CAD systems, we present a new method for reverse engineering of materials such that models of material microstructure can be constructed and used as CAD representations to support heterogeneous part modeling. Such material models capture microscopic features and enable integration with structure–property relationships. Furthermore, these models are based on wavelet basis functions which support multi-resolution representations. The proposed method uses a new surfacelet–wavelet representation to efficiently capture internal and boundary information implicitly [1].

The proposed method for reverse engineering of materials is shown schematically in Fig. 1. A material sample is sliced and imaged at appropriate resolutions to capture its microstructure and enable construction of process–structure–property relationships at the smallest size scale of interest. Before image analysis, the user specifies material compositions (i.e., which colors or shades correspond to which materials). Image analysis is performed to extract the geometry of the material's microstructure (e.g., grain or particle size, shape, orientation) and correlate it with material compositions. Image analysis is comprised of three main steps, (1) a Radon-like surfacelet transform and (2) a wavelet transform, which results in a surfacelet model of microstructure and material composition, then (3) a feature recognition algorithm. The Radon transform is an effective method for representing line singularities in 2D and 3D images [2] (i.e., finding straight edges in images). The Radon transform was developed to reconstruct images from CT scans [3], which consist of sets of parallel scans where the source and sensor rotate around the target. The wavelet transform enables multi-resolution models of microstructure to be computed. Microstructure features are recognized by identifying peaks in the

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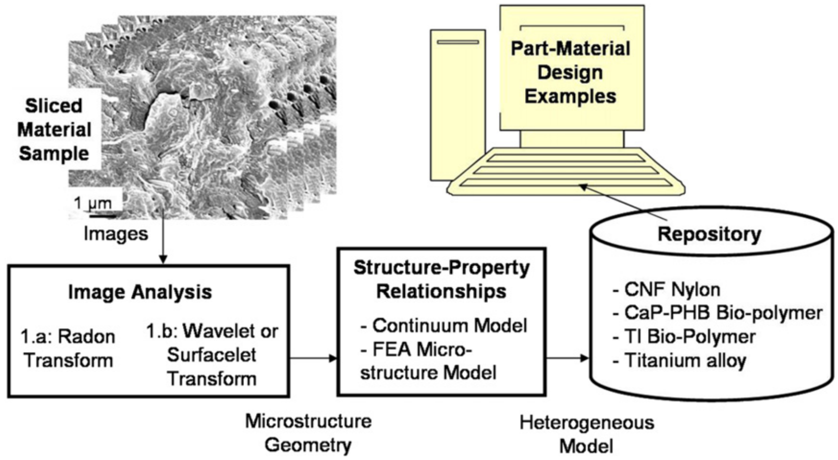

Fig. 1. Proposed reverse engineering of materials process.

high frequency part of the wavelet transform matrix, finding clusters of those peaks, and selecting the highest peak in each cluster.

Such a microstructure model enables integration with material process–structure–property relationships in order to determine properties of interest. For example, a material's elastic modulus and Poisson's ratio can be estimated from finite-element analysis. From the microstructure, process–structure relationships can also be determined. Multiscale models will be enabled through the multi-resolution capabilities of wavelet and surfacelet functions that we use to represent microstructure geometry. As a result, we will have the capability of constructing multiscale, heterogeneous models of materials that can be integrated into CAD systems and used for mechanical part design. This concept is similar to the geometric modeling methods and multiscale finite-element analysis capability that other researchers developed for bone [4]. Our objective is to extend these types of capabilities to a wide variety of other engineering materials.

In this paper, we will focus on the generation of surfacelet models of material microstructure. In contrast, in an earlier paper [1] we discussed the representation of material distributions and microstructures by first specifying materials and properties at a finite number of positions. In the remainder of the paper, we begin with a brief background review of Radon, wavelet, and surfacelet transforms in Section 2. In Section 3, feature recognition from images based on the surfacelet transform is described. This reverse engineering approach is applied to three examples in Sections 4–6.

2. Background

In this section, we give a brief overview of relevant work to our proposed reverse engineering of materials approach, including heterogeneous modeling in Section 2.1 and surfacelet models in Section 2.2, including Radon and wavelet transforms.

2.1. Heterogeneous modeling

Heterogeneous modeling usually denotes the modeling of geometry and material composition. Kou and Tan [5] recently surveyed the field and identified three broad categories of research: evaluated, unevaluated, and composite approaches. Evaluated representations are inexact and are based on discretizations, where materials and geometry are modeled separately using mesh-based and voxel-based methods [6] or general cellular decompositions [7]. In unevaluated approaches, some researchers have separated the representation of material compositions and properties from the underlying part geometry [8]. Others have utilized implicit modeling approaches, which have advantages in that a common mathematical model is used for both geometry and material composition [9,10]. In composite methods, the part is decomposed into several sub-objects, each of which belongs to a different material class, which may be evaluated or unevaluated [11]. Objects constructed using Boolean operations [6] or modeled using cellular methods fall into this category [7].

The common limitation is that the approaches specify material compositions using constant or continuous distributions (typically using parameterizations) that are not based on the actual material behavior and do not honor the material's physics. In contrast, our proposed approach is focused on understanding material microstructure and associating microstructure features with material compositions and mechanical properties. That is, our material models can be integrated with process–structure–property relationships that can then be integrated into CAD models.

2.2. Surfacelet models

As introduced in [1], surfacelet models can be generated by a combination of Radon-like surfacelet and wavelet transforms. In this paper, we only consider the Radon transform, a special case of surfacelet transform, in the analysis. The Radon and wavelet transforms will be summarized here.

2.2.1. Radon transform

The Radon transform is based on integrals over straight lines. The mathematics of Radon transforms describes the imaging operations of CT scanners in which X-ray sources emit a set of parallel X-rays at multiple angles around the object to be imaged [3]. The inverse Radon transform is used to reconstruct the original image from the sensor data obtained during the imaging step. Since the Radon transform is based on integrals over straight lines, if geometric features with linear geometry exist in the object to be imaged, those linear features can be recognized readily. This capability has been used in many applications in image compression [2], image reconstruction [12], and feature recognition [13,14]. The Radon transform is closely related to the Hough transform; the complex Hough transform has been used to recognize grains in 3D alloy microstructure datasets [15].

The Radon transform of a 2D image is defined by the integral along a line, L, as

$$R_f(L) = \int_L f(\mathbf{x})\,|d\mathbf{x}| \quad (1)$$