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Simulation of residual stress and elastic energy density in thermal barrier coatings using fast Fourier transforms

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ABSTRACT

A numerical method for solving the thermoelastic problem in heterogeneous polycrystals based on fast Fourier transforms is applied to thermal barrier coating systems. Several high resolution microstructures are generated synthetically to approximate thermal barrier coatings, with control over the grain size, grain morphology, and texture. Interfaces between coating layer materials are further modified by applying a localized Potts model to introduce interface rumpling. The global results of residual stress and elastic energy density are compared across the various microstructure instantiations. The local variations in elastic energy density are correlated to the amount of interface rumpling. The simulation result are also compared to an analytical result for an idealized interface morphology. The implications of the behavior of the local variations in elastic energy density are discussed in the context of thermal barrier coating failure.

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1. Introduction

Structural metallic components operating in gas turbine engines are often exposed to extreme levels of temperature [1,2]. In such systems, it is desirable to increase the operating temperature, thereby improving efficiency and performance [3,4]. However, the mechanical properties of the metallic component must remain constant at elevated temperatures to avoid the potential for failure [5]. In order to provide insulation and protection for the metallic component, it is common to apply a ceramic coat to the metallic surface in contact with the combustion gas. These thermal barrier coating (TBC) systems, along with sufficient internal cooling, are capable of reducing the surface temperature of the alloy up to 100 °C [6]. This allows operating temperatures above the melting point of the metallic component (~1300 °C for a nickel based superalloy) [6].

TBC systems consist of several layers, including the structural metallic substrate, a metallic bond coat (BC), a ceramic thermally grown oxide (TGO), and a ceramic top coat (TC). The entire TBC system is subject to extreme variations in temperature, resulting in the development of significant thermal residual stresses attributed to the thermal expansion mismatch between layers and the intrinsic anisotropy in each layer [7,8]. These residual stresses can lead to the development of defects at the interfaces between constituent TBC layers known as "rumpling" [9–11]. The rumpling is a result of the TGO attempting to relax the strain energy associated with its intrinsic residual stress. Due to the thermal expansion mismatch between the BC and TGO, the TGO will develop compressive stresses within the plane normal to the interface on cooling [10,11]. To accommodate these residual stresses, the TGO will attempt to lengthen itself by displacements out of the interface plane [6,9]. The resulting stresses will then redistribute around the rumpling features [9,10]. The undulations may also continue to grow via a process known as "ratcheting" [9,12]. The growth of such interface features causes stress localization, eventually leading to cracking at the BC/TGO or TGO/TC interfaces. The source of the macroscale cracking is thus tied to a microstructurally local phenomenon.

Experimental assessment of TBC failure is essential for determining a limiting lifetime for components, but does little to reveal the local origins of failure [13–16]. Additionally, nondestructive measurements of residual stress are generally restricted to the macroscale [17,18]. Modeling provides an opportunity to investigate local residual stresses in TBC systems. In the present analysis, we utilize a spectral approach based on fast Fourier transforms (FFTs) to solve the constitutive equations related to thermal

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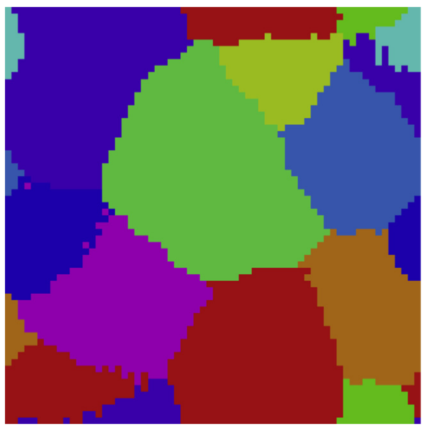
residual stress. This approach provides the possibility for $\mathcal{O}(n \log n)$ scaling, where n is the number of nodes utilized in the simulation [19]. Comparable finite element methods (FEM) generally scale as $\mathcal{O}(n^2)$ and require a meshing procedure, inevitably leading to overall longer compute times. Since the present technique is image based, no meshing is needed, allowing for complex microstructures to be assessed.

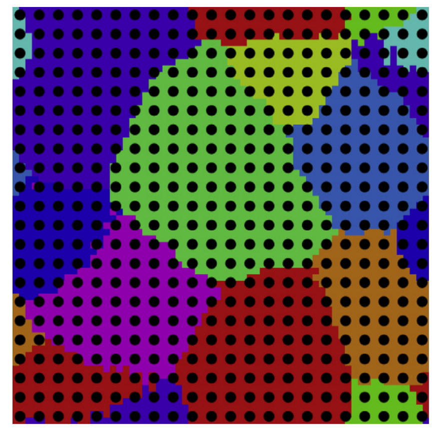
2. The thermoelastic FFT method

In classical linear elasticity, stress and strain are related via Hooke's Law:

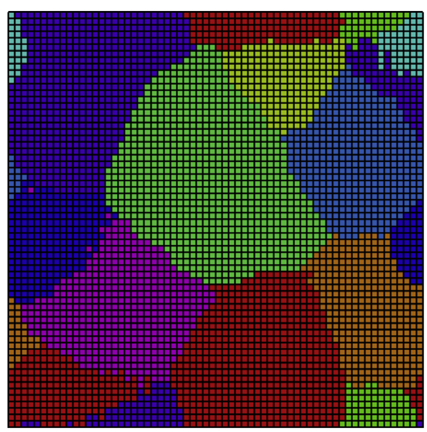
$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} \tag{1}$$



(a) Underlying sample microstructure.



(b) Overlay of rectilinear grid.



(c) Center-weighted pixelization.

Fig. 1. A sample discretized 2D microstructure suitable for use as input to the thermoelastic FFT code.

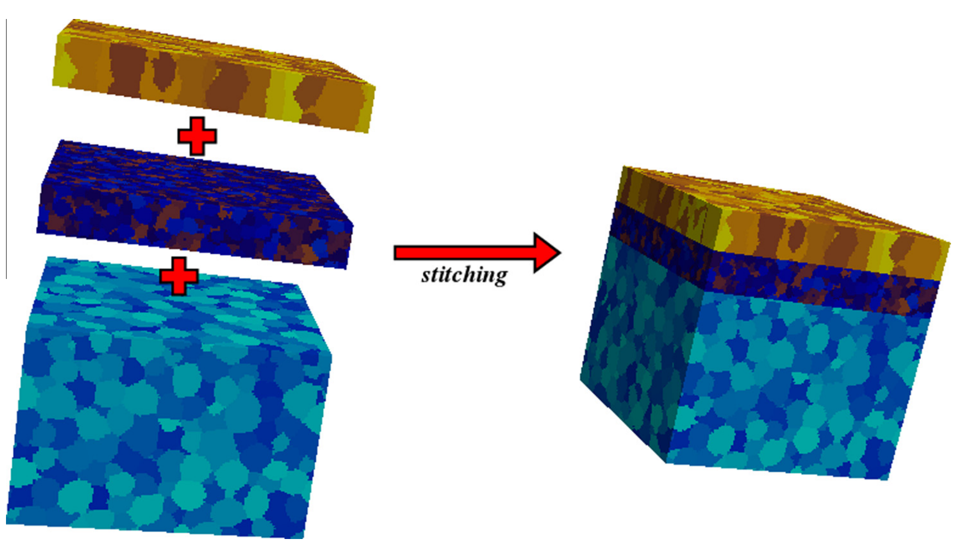


Fig. 2. Stitching process used to create layered thermal barrier coating microstructures.

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