Computational study of oxidative etch pitting in FiberForm and the effect on its material properties.

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Abstract

Erosion of carbon due to oxidation does not occur uniformly but through the formation of localized etch pits because of active surface sites [1]. These active sites are formed due to the presence of atomic defects on the carbon surface, and have much higher reactivity compared to average non-defective sites. Thus, these active sites are first to react during ablation, resulting in their removal. This causes all the neighboring atoms to be defective and increase their reactivity, thus leading to the localized carbon removal around these "active" sites. In this manner, these highly reactive defective sites serve as nucleation sites for the formation and growth of etch pits [2] with potentially detrimental effects on the structural integrity.

In order to understand the influence of these etch pits on the material properties of carbon fiber microstructures, we have developed a new capability within direct simulation Monte Carlo (DSMC) to capture the etch pit formation process. This capability is developed within the DSMC code SPARTA (Stochastic PArallel Rarefied-gas Time-accurate Analyzer) [3] and can model the material removal in presence of active sites leading to the formation of etch pits. The focus of the current work will be to study the effect of etch pits on the material properties of FiberForm, a commonly used base material within many thermal protection system materials (TPS). The microstructure of virgin FiberForm obtained directly from X-ray microtomography experiments [1] is used within SPARTA to obtain the ablated geometries with etch pits (as shown in Fig. 1). These pitted microstructures are then imported within the Porous Microstructure Analysis (PuMA) software [4] and various material properties such as elasticity, thermal conductivity, and permeability are computed.

The variation of these properties as a result of the complex evolution of the surface topology due to etch pit formation is studied and analyzed. Furthermore, the effect of pitting is compared to the case of shrinking fibers, which has been the standard for modelling ablation of carbon structures; and significant differences are observed. Thus, such a physically realistic modeling of material removal through the formation of etch pits will be helpful in predicting the degradation of carbon-based TPS more accurately during oxidation; as well as other mechanisms such as spallation, which involves the removal of chunks of material into the flow due to etch pit growth. This will ultimately improve our understanding of the failure modes in these materials due to ablation.

Keywords: Carbon Ablators, Oxidation, Etch Pitting, Microstructure, PuMA, SPARTA, DSMC.

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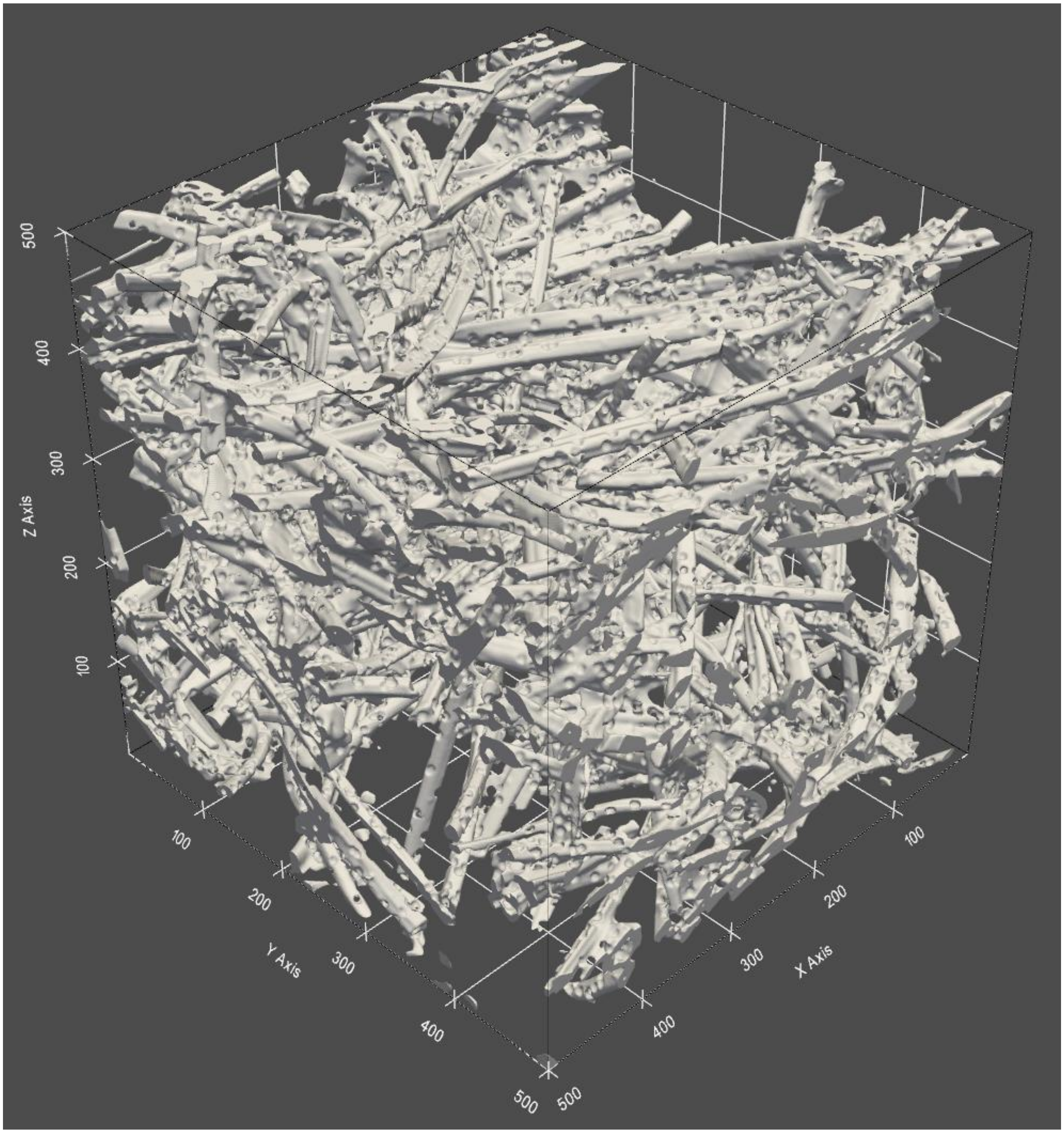

Figure 1: FiberForm sample with oxidative etch pits obtained from SPARTA and used within PuMA to compute various material properties.