Formation, structure and properties of amorphous carbon char from polymer materials in extreme atmospheric reentry environments

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Amorphous carbonaceous char produced from the pyrolysis of polymer solids has many desirable properties for ablative heat shields for space vehicles. Molecular dynamics simulations are presented to study the transformation of the local atomic structure from virgin polymer to a dense, disordered char [1]. Release of polymer hydrogen is found to be critical to allow the system to collapse into a highly coordinated char structure. Mechanisms of the char formation process and the morphology of the resulting structures are elucidated. Thermal conductivity and mechanical response of the resulting char are evaluated [2]. During reenty, the optical response and oxidative reactivity of char are also important properties. Results of *ab initio* computations of char optical functions [3] and char reactivity [4] are also presented.

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