

COMPUTATIONAL CHEMISTRY MODELLING OF THE OXIDATION OF HIGHLY ORIENTED PYROLYTIC GRAPHITE

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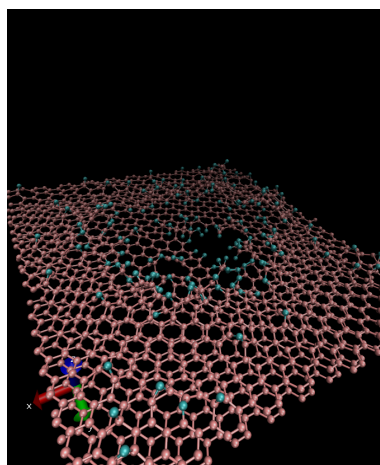
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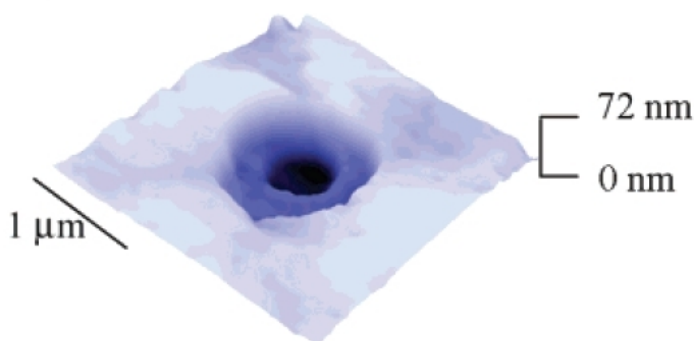
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Under high heat flux, carbon based Thermal Protection Systems (TPS) are observed to rapidly ablate and an accurate characterization is essential to their design. Dissociated oxygen atoms (from the gas phase) striking the surface of TPS could lead to several possibilites. The O atom could adsorb on the surface, recombine with another O atom to form O₂ and oxidize the surface to produce CO or CO₂ resulting in recession of the surface (ablation). The goal is to predict finite rate models for these reactions which could be incorporated into CFD and DSMC solvers. Our efforts are to predict the rates through large scale Molecular Dynamics (MD) simulations using the ReaxFF potential which enables accurate simulation of large chemically reacting systems of molecules. In this work, we simulate the collision of hyperthermal (5eV) O atoms on Highly Oriented Pyrolytic Graphite (HOPG) at 525K. The simulations are compared to molecular beam experiments performed by Minton[1] and co-workers.

The simulations predict the pit growth in the intraplanar direction to be much more rapid than etching in the interplanar direction. This was observed experimentally (Fig. 1) where shallow but wide etch pits were created. The experimental results predict the probability of oxidation (removal of carbon atom) in the prismatic plane (intraplanar direction) at about 0.44 (roughly 1 carbon atom for 2.3 O atoms) and our results predict that about 1 carbon atom is removed for every 5.96 O atoms. The simulations have reasonable quantitative and qualitative agreement with experimental results. Results of the surface temperature dependence on etching rate will also be presented.



(a) Surface of HOPG after O atom collisions from simulation. Only top 2 layers shown



(b) Surface of HOPG after O atom collisions from experiments

Figure 1: The figure compares the surface of HOPG after collisions with O atoms at 5 eV from both simulations and experiments.

1. REFERENCES

- [1] Nicholson K.T., Minton T.K., Seibner S.J., Spatially Anisotropic Etching of Graphite by Hyperthermal Atomic Oxygen, J Phys. Chem B 2005, 109.