Multi-scale Study of Nuclear Graphite Oxidation with Oxygen: Reactive sites ratio derivation

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Nuclear grade graphite oxidation is a multi-length scale study, it couples the chemical kinetics, heat and mass transport, and porous structure evolution issues, and physically includes five levels of observation: graphene plane edge sites reactions, crystallite structure effects-multiple layers of graphene, crystallites shielding-assembling of randomly oriented crystallites, microstructure evolution-pores development, and component level corrosion-a couple of chemical reactions, heat and mass transfer.

It's difficult to understand every level of graphite oxidation theoretically and thoroughly, but it is important to realize the connections and evolutions of each level oxidation, which helps us to understand the wide varied oxidation rates and establish a fundamental model for the graphite-oxygen oxidation system independent of graphite grades, then apply it for new nuclear graphite under any circumstances.

Significant variables of this model while applying it to different graphite are the total surface area (TSA), active surface area (ASA) and reactive surface area (RSA). The ratios of ASA and RSA to TSA are calculated by equations derived from few ideal shapes of graphene plane. We calculated the ratios on more shapes of planes, and derived a refined equation which could help us to understand how edge sites affect the oxidation and the differences between graphite grades.