

Monte Carlo Computational Modeling of Atomic Oxygen Interactions

Bruce A. Banks¹
Thomas J. Stueber²
Sharon K. Miller²
Kim K. de Groh²

¹SAIC at NASA Glenn Research Center

²NASA Glenn Research Center

The Monte Carlo model described is a two dimensional atomic oxygen interaction model that predicts erosion of an oxidizable material under a non-reactive layer with an opening in it. Erosion is by direct arrival and by scattering inside the forming cavity. In the model, the oxidizable material, such as a polymer like Kapton H polyimide, is divided into millions of small mathematical envisioned cells that are covered by a non-reactive layer, such as silicon dioxide, that has a crack opening in it. The model predicts the shape of the eroded polymer as a result of oxidation from atomic oxygen impact that can be of any energy ranging from hyperthermal energy characteristic of low Earth orbit to thermal energy representative of radio frequency plasma ashers. This specific geometry was chosen because it allows all the needed atomic oxygen interaction parameters to be tuned to match actual space results, thus allowing a wide variety of geometries to be considered for atomic oxygen interaction predictions.

In the model oxygen atoms are injected into an opening in the crack where upon they can react, recombine, or scatter. To start the model one must be able to describe the atomic oxygen energy, the angle of attack, the energy distribution, and the cumulative fluence. The location and direction of impact of oxygen atoms is randomly selected based on whether the surface is maintained in a ram facing direction or has sweeping arrival such as on the International Space Station solar arrays.

For ram facing surfaces, the energy and angle of impact is a result of the vectoral addition of orbital velocity, a reduction of the orbital velocity due to the co-rotation of the Earth's thermosphere, and the random Maxwell Boltzmann thermal velocity distribution. The resultant total velocity vector varies slightly in energy and direction around each orbit because of the variation of the co-rotational velocity with latitude. This variation along with the Maxwell Boltzmann thermal velocity distribution gives the arriving flux somewhat of a search light distribution in that all the oxygen atoms do not arrive in a paraxial manner. Even at 180 degrees from the ram direction, the hot tail of the Maxwell Boltzmann distribution allows some oxygen atoms to catch up to the spacecraft even though their numbers are many orders of magnitude below that of the number arriving from the ram direction. At 90 degrees from the ram direction there is ~ 4.15% of the ram flux arriving as a result of arrival distribution variations. The energy of the impacting atomic oxygen goes down with increasing altitude due to the subtraction of the co-rotation velocity vector and the lower ram orbital velocity (Ref. 1).

Atomic oxygen interactions are mostly relevant only for altitudes below 650 km due to the number density dropping off so quickly with increasing altitude. This would, of course, be different from atomic oxygen in a Martian orbit. In Earth orbit, the average atomic oxygen flux

peaks at orbital altitudes of 100 km where it imposes an enormous drag on a spacecraft then gradually drops off with altitude.

Upon initial impact of an atomic oxygen with a material there is a variety of possible interaction possibilities that the Model simulates. It can: 1) react resulting in removal of a Monte Carlo cell; 2) not react and be scattered away from the surface it hits and possibly impact another cell or be ejected out the opening; or 3) recombine with a previous atomic oxygen atom that is temporarily attached to a surface and form passive diatomic oxygen. Any scattered oxygen atom can partially or fully thermally accommodate thus reducing its reaction probability. Most of the same interaction processes (with the exception of reacting) can occur if the atomic oxygen impacts a non-reactive surface.

Each of these interaction processes have their own probabilities of occurring which can be estimated by careful measurement of actual low Earth orbital atomic oxygen erosion at sites of crack defects on protected polymers as well as erosion of multilayer polymers.

The reaction probability appears to be dependent upon the cosine of the angle of impact raised to the 0.5 power based on retrieved data from the LDEF spacecraft (Ref. 2). Based on retrieved atomic oxygen erosion data, a reaction probability dependent upon the activation energy of the 0.26 eV has produced the closest match between observed undercut profiles and Monte Carlo modeled profiles. Scattered oxygen atoms have different fractional recombination probabilities, degrees of specular versus diffuse ejection patterns, and different fractional energy loss depending upon whether the surface is a reactive surface or a non-reactive surface. There are other assumptions that need to be made which can also be calibrated to cause the model to produce erosion predictions that match actual in-space results. In total there are about 15 interaction parameters that can be optimized to cause the Monte Carlo model to agree with a variety of known space results. It is likely that there may be more than a single set of interaction parameters that satisfy a match with space results but the more results that are compared, the more likely to narrow in on a single set of parameters.

Figure 1 shows how some of the in-space results of atomic oxygen erosion of a crack defect in an aluminized coating on Kapton H were used to tune of the interaction parameters such that the Monte Carlo model predicted patterns that matched space results (Ref. 3). The little bump on the top left wall of the eroded cavity, shown in Figure 1d, is the result of atomic oxygen scattering off the opposing edge of the protective coating on the right because the atomic oxygen arrival was 8.1 ° off normal.. In this particular model each Monte Carlo cell represents 8.28×10^{-13} cm with each Monte Carlo atom represents $\sim 2 \times 10^9$ atoms.

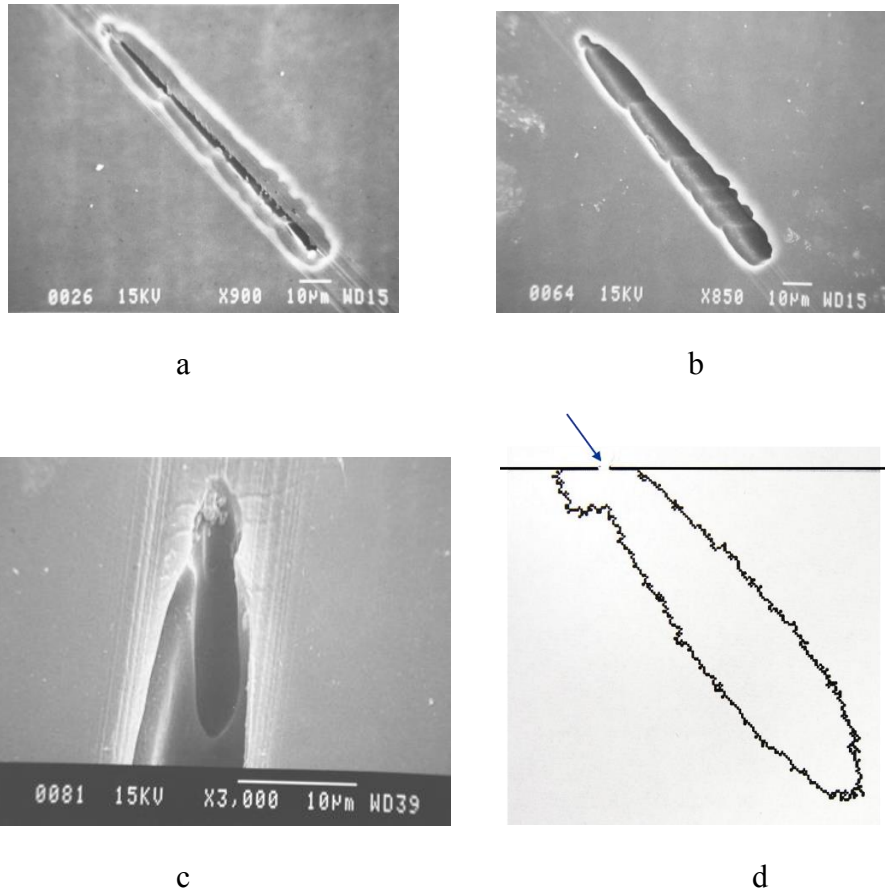


Figure 1. Retrieved Long Duration Exposure Facility sample of aluminized Kapton H polyimide and a Monte Carlo computational model simulation. a – aluminized Kapton sample as retrieved, b – after chemical removal of cracked aluminum coating, c – image of undercut cavity rotated for measurement purposes. d – Monte Carlo model prediction.

The space results comparing separated multilayer polymers polymer erosion with single layer polymers was also used to tune the Monte Carlo modeling interaction parameters to enable predictions of erosion that agree with space results (Ref. 3).

One of the indications of the success of the Monte Carlo model is that it predicts the same texturing that is actually produced in space for ram atomic oxygen attack of all hydrocarbon and halocarbon polymers. The texturing grows as the square root of the fluence which is consistent with Poisson statistics where spatially independent sites of erosion evolve into left-standing cones (Ref. 4). A Monte Carlo prediction has been used to explain why the double-coated aluminized Kapton blanket box covers eroded quickly on the International Space Station solar arrays. The model shows that it is due to trapped atomic oxygen at sites of pin window defects. It also shows that if the aluminization was just on the exposed surface there would have been greater durability of the blanket because trapping would not have occurred. The Monte Carlo model interaction parameters relating to scattering off reactive and non-reactive surfaces also allows quantified prediction of scattered atomic oxygen fluences at locations within spacecraft such as telescope openings where there may be sensitivity of materials inside to atomic oxygen attack or erosion (Ref. 5).

This presentation describes the Monte Carlo model, parameters for determining erosion, and gives examples of its use for durability prediction.

References

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