Monte Carlo Computational Modeling of Atomic Oxygen Interactions

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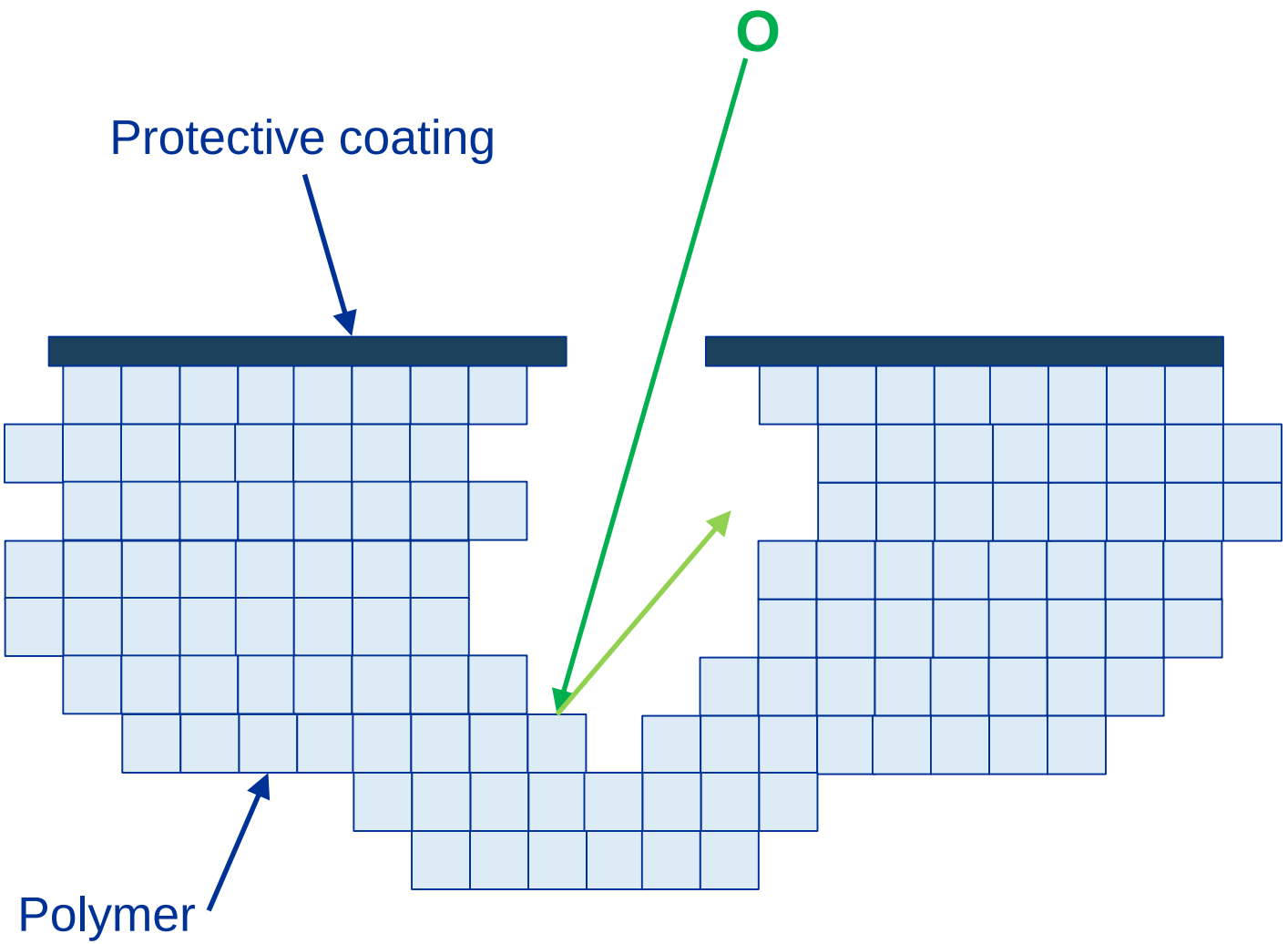
2-D Monte Carlo Computational Model



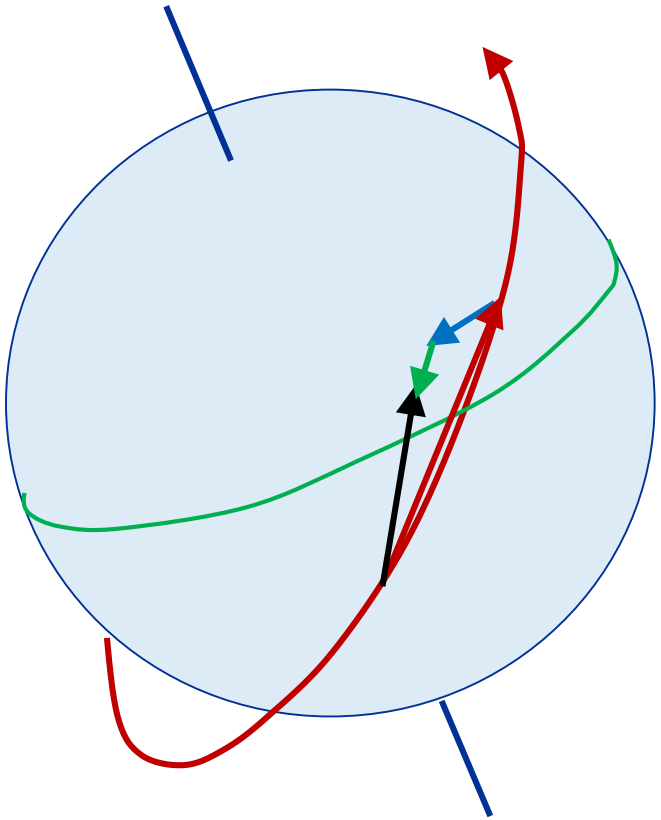
Arriving Atomic Oxygen Characteristics

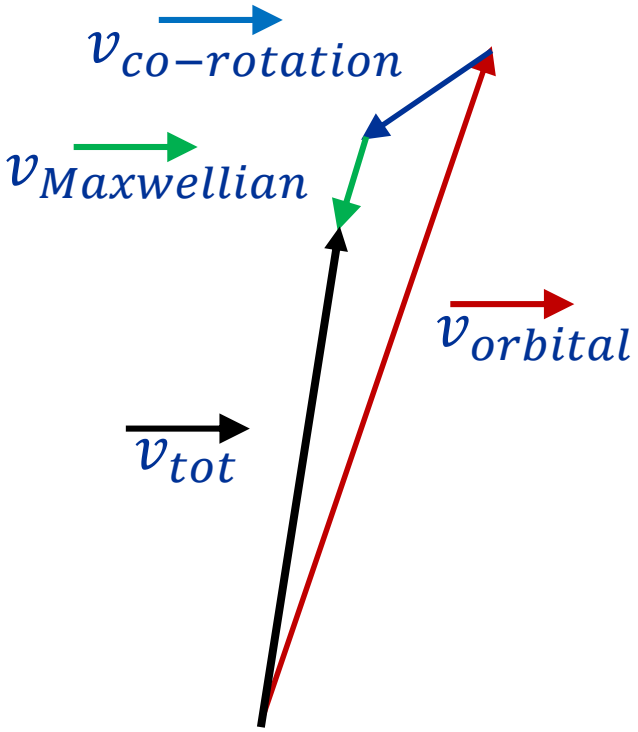
- Energy
- Angle and position of attack
- Averages over each orbit
- Fluence

Atomic Oxygen Energy

$$\vec{v}_{tot} = \vec{v}_{orbital} + \vec{v}_{co-rotation} + \vec{v}_{Maxwellian}$$

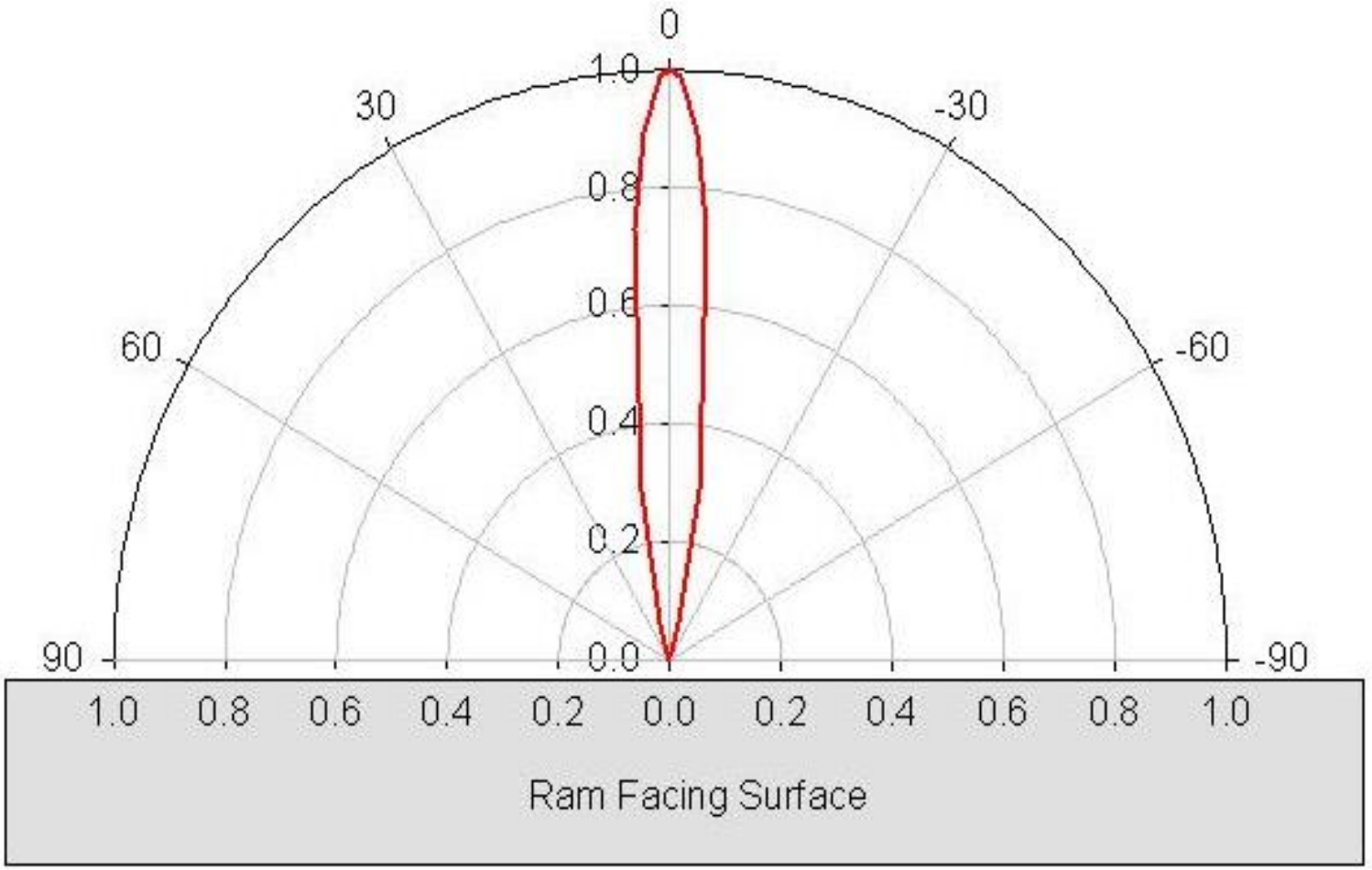
7.9 Km/sec 0.49 Km/sec 0.41 Km/sec



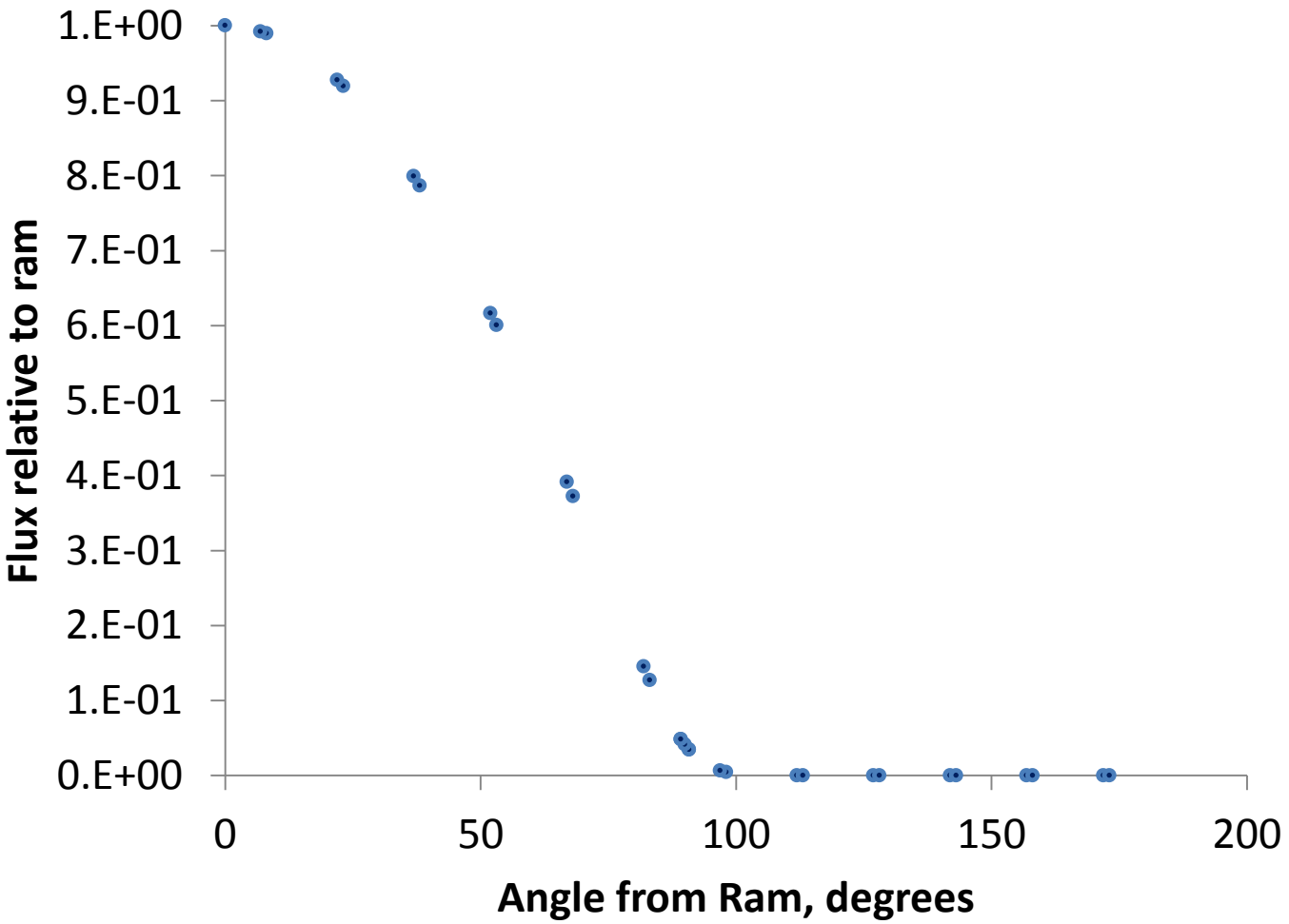


Atomic Oxygen Flux vs Angle from Ram

at 400 km orbit and 28.5° inclination and 1000K thermosphere

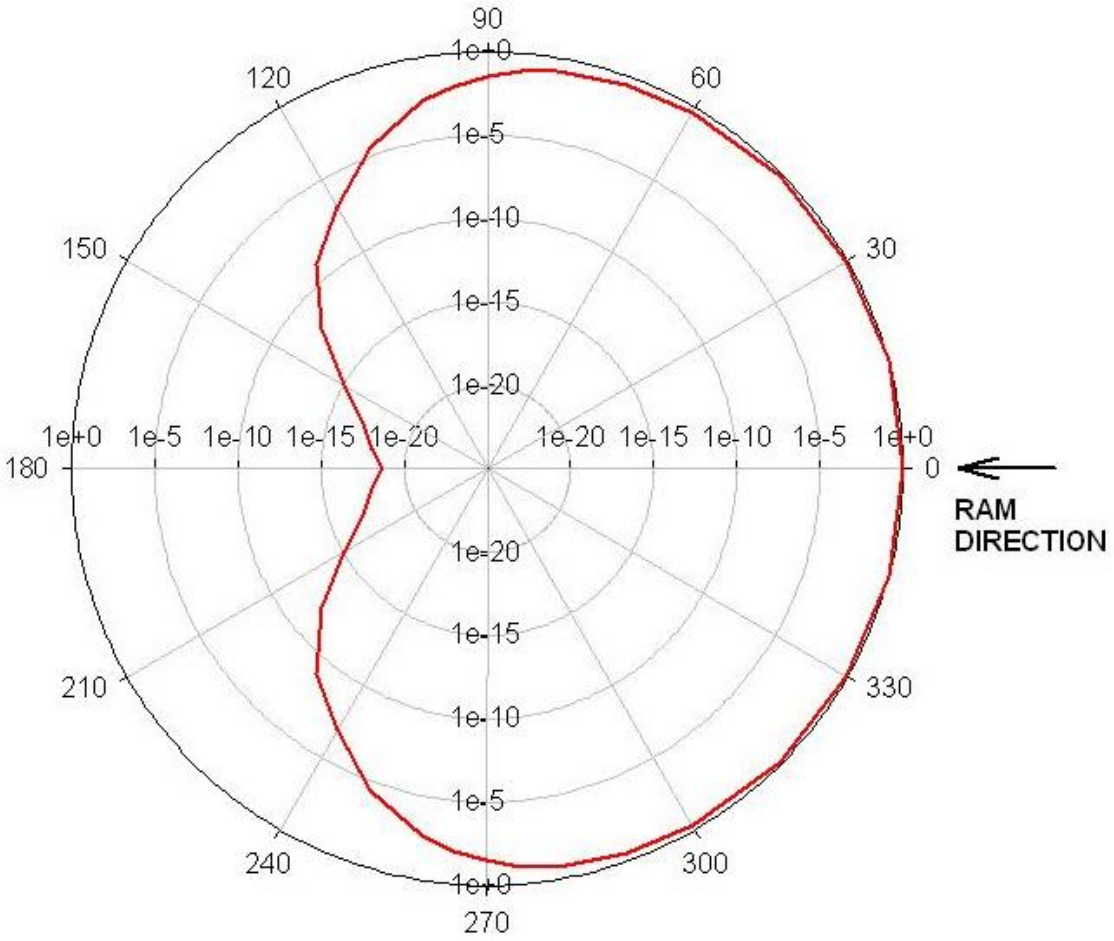


Atomic Oxygen Flux vs Angle from Ram



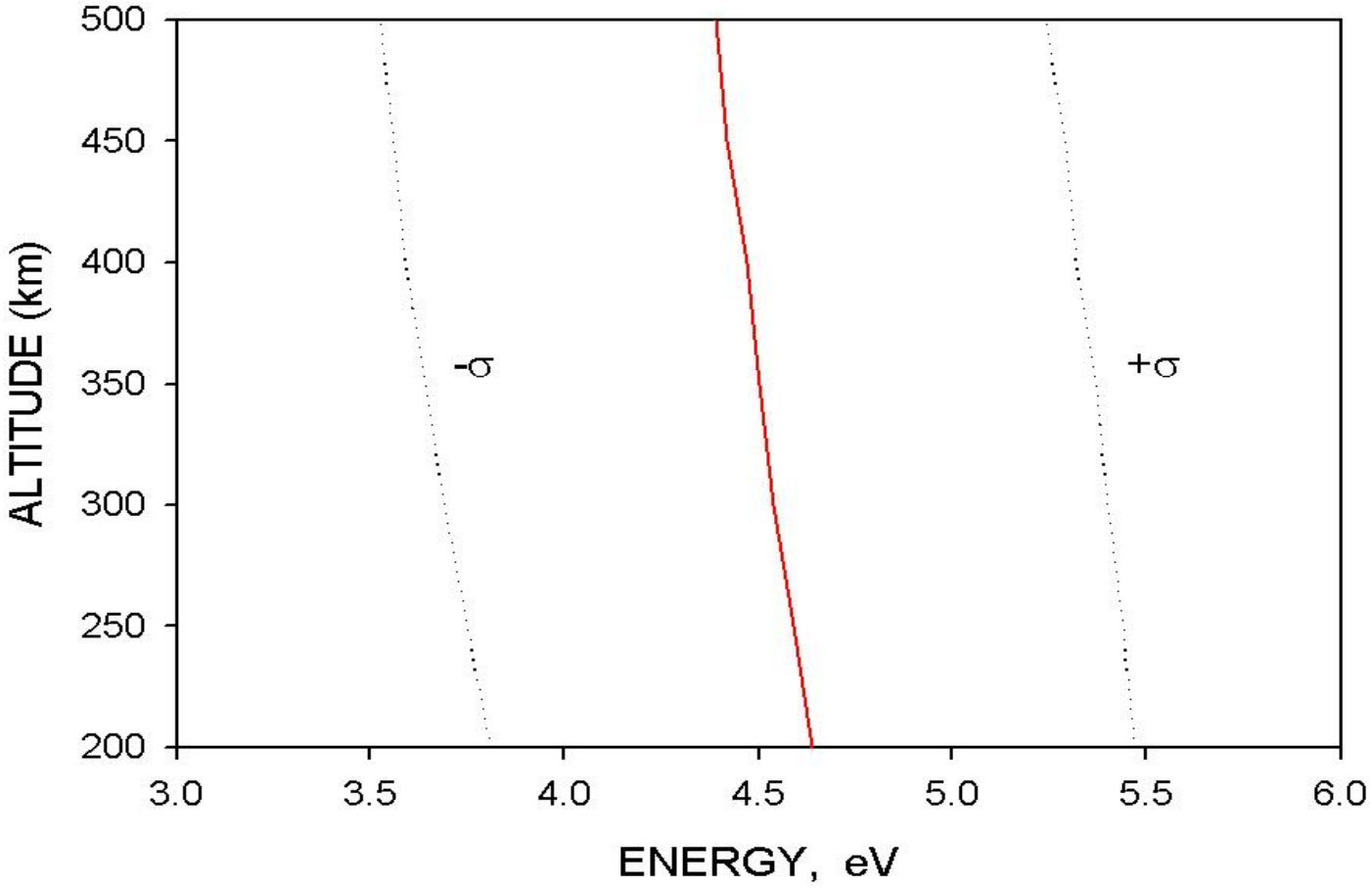
Atomic Oxygen Arrival Direction

at 400 km circular orbit

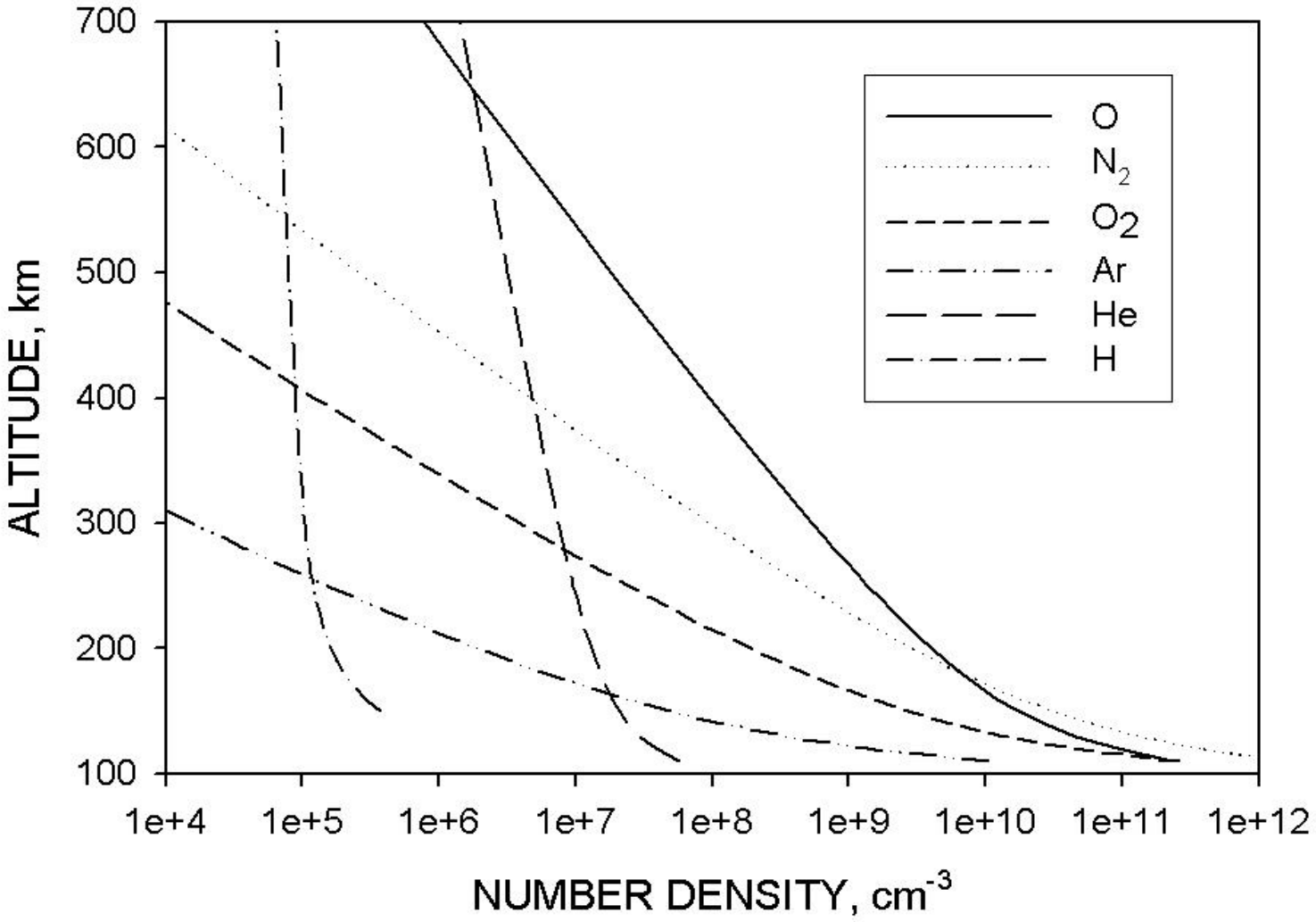


Atomic Oxygen Energy Versus Altitude

at 400 km circular orbit, 28.5° inclination

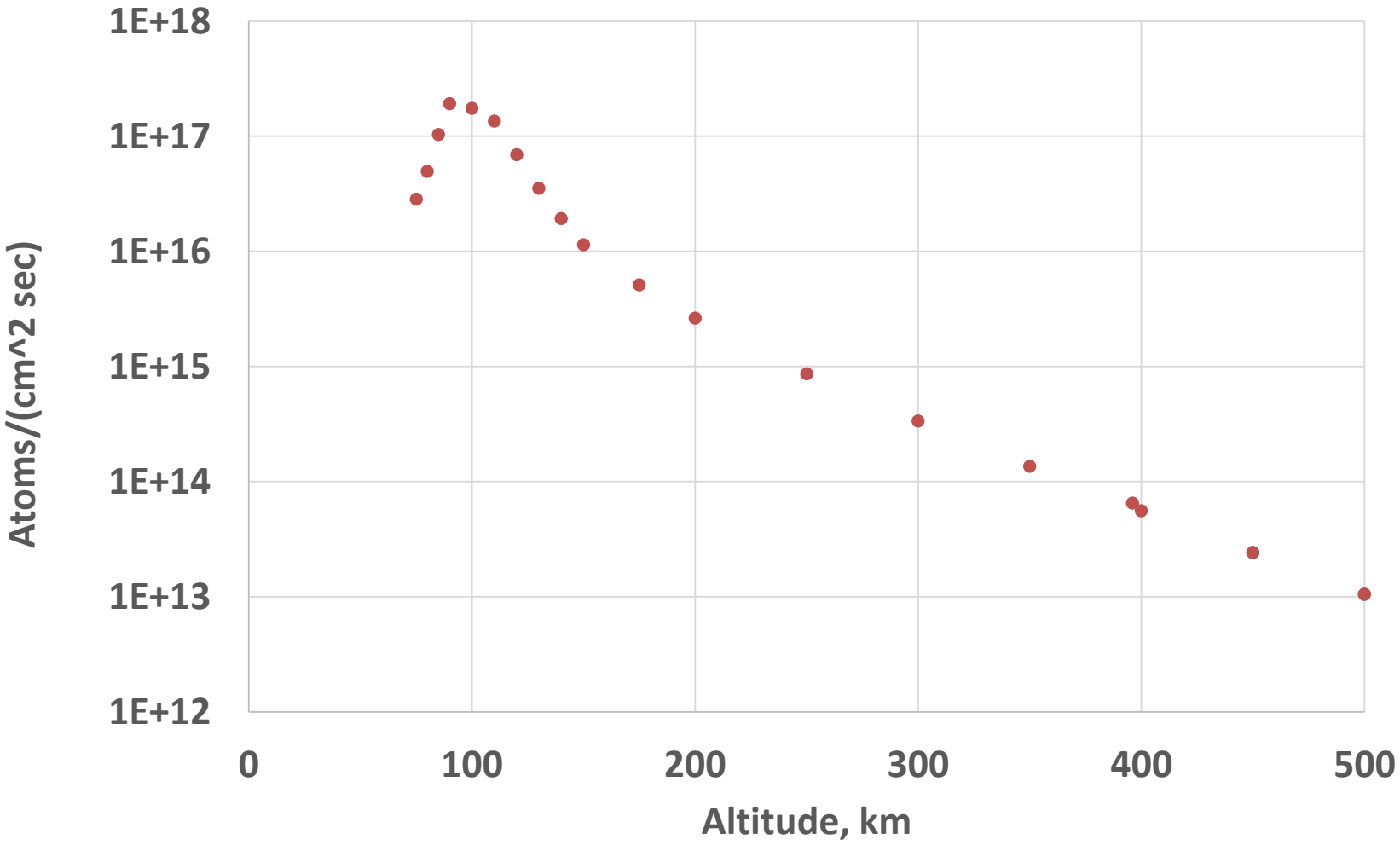


Atomic Oxygen Number Density Versus Altitude



Atomic Oxygen Flux Versus Altitude

Averaged over a solar cycle for a 96 degree inclined circular orbit



Atomic Oxygen Interaction Characteristics

- Initial impact
  - Reactive surface
    - React and remove a cell
    - Scatter away from the impacted cell
    - Recombine to form O_2
    - Partially thermally accommodate
  - Non-reactive surface
    - Recombine to form O_2
    - Scatter away from the impacted cell
    - Partially thermally accommodate

Upon Initial Atomic Oxygen Impact
for a 2D model

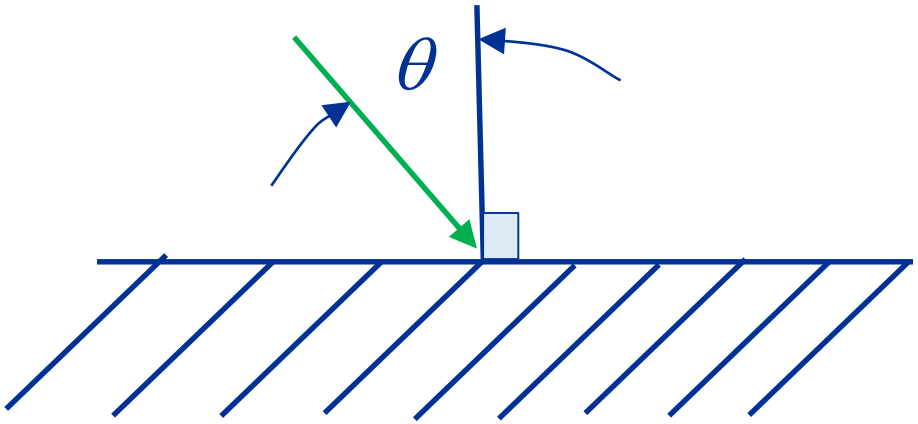
- **Randomly select location and direction of impact**
  - Fixed direction
  - Sweeping direction

- **Reaction probability dependence upon angle of impact**

$$P_C = (\cos\ \theta)^n$$

Where θ = the angle between the arriving atomic oxygen direction and the local surface normal

n = cosine exponent = 0.5 based on optimization



Upon Initial Atomic Oxygen Impact
for a 2D model

- **Off reactive surfaces**
- **Energy dependent reaction probability**

$$P_E = ce^{-E_A/E}$$

Where c = 3.178 x 10^{-24}

E_A = activation energy = 0.26 eV based on optimization

E = atomic oxygen impact energy, eV = 4.5 eV

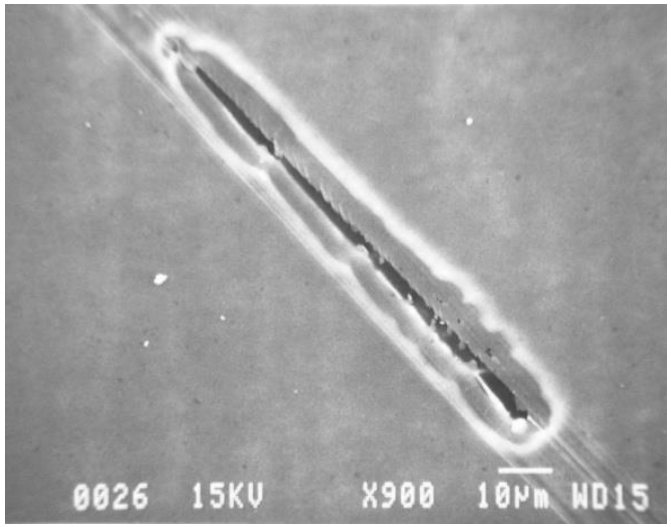
Scattering of Atomic Oxygen
for a 2D model

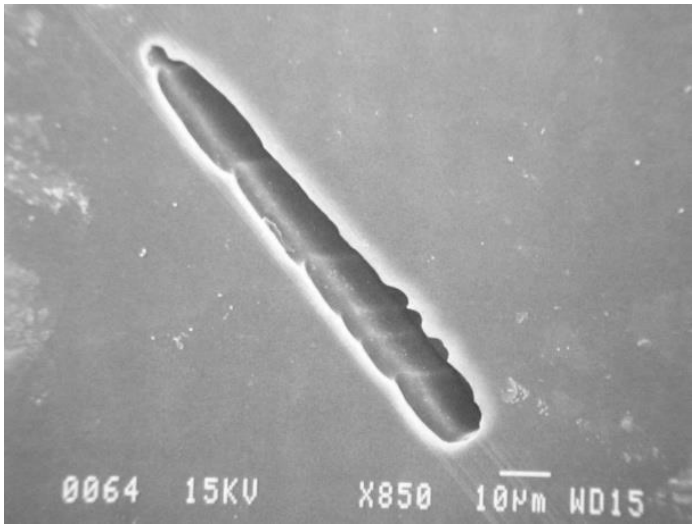
Scattering Description	Off Reactive Surfaces	Off Non-Reactive Surfaces
Fractional recombination	0.3	0.33
Degree of specular as opposed to diffuse ejection	0.2	0.5
Fractional energy loss upon ejection	0.4	0.05

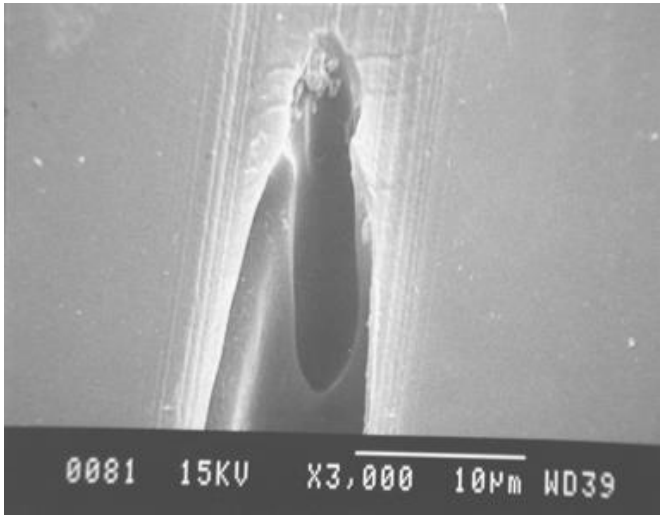
Other Monte Carlo Computational Assumptions

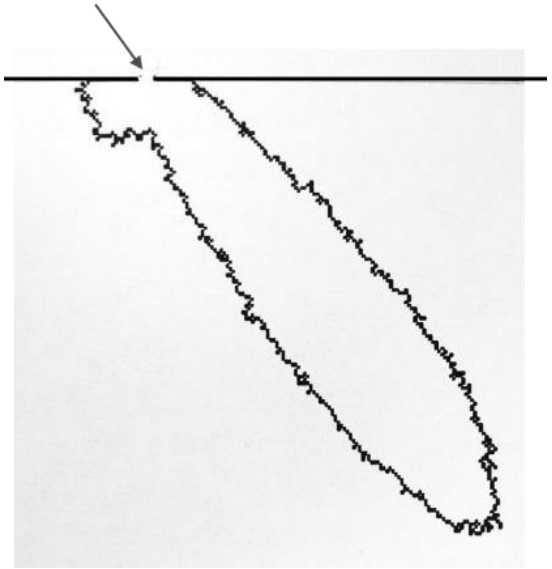
Temperature for thermally accommodated atomic oxygen atoms, K	300
Limit of how many bounces the atomic oxygen atoms are allowed to make before an estimate of the probability of reaction is assigned	25
Thermally accommodated energy/actual atom energy for atoms assumed to be thermally accommodated	0.9
Initial atomic oxygen energy, eV	4.5
Thermospheric atomic oxygen temperature, K	1000
Atomic oxygen arrival plane relative to Earth for a Maxwell-Boltzmann atomic oxygen temperature distribution and an orbital inclination of 28.5^{o}	Horizontal

Monte Carlo Modeling of 2D Crack in Al on LDEF

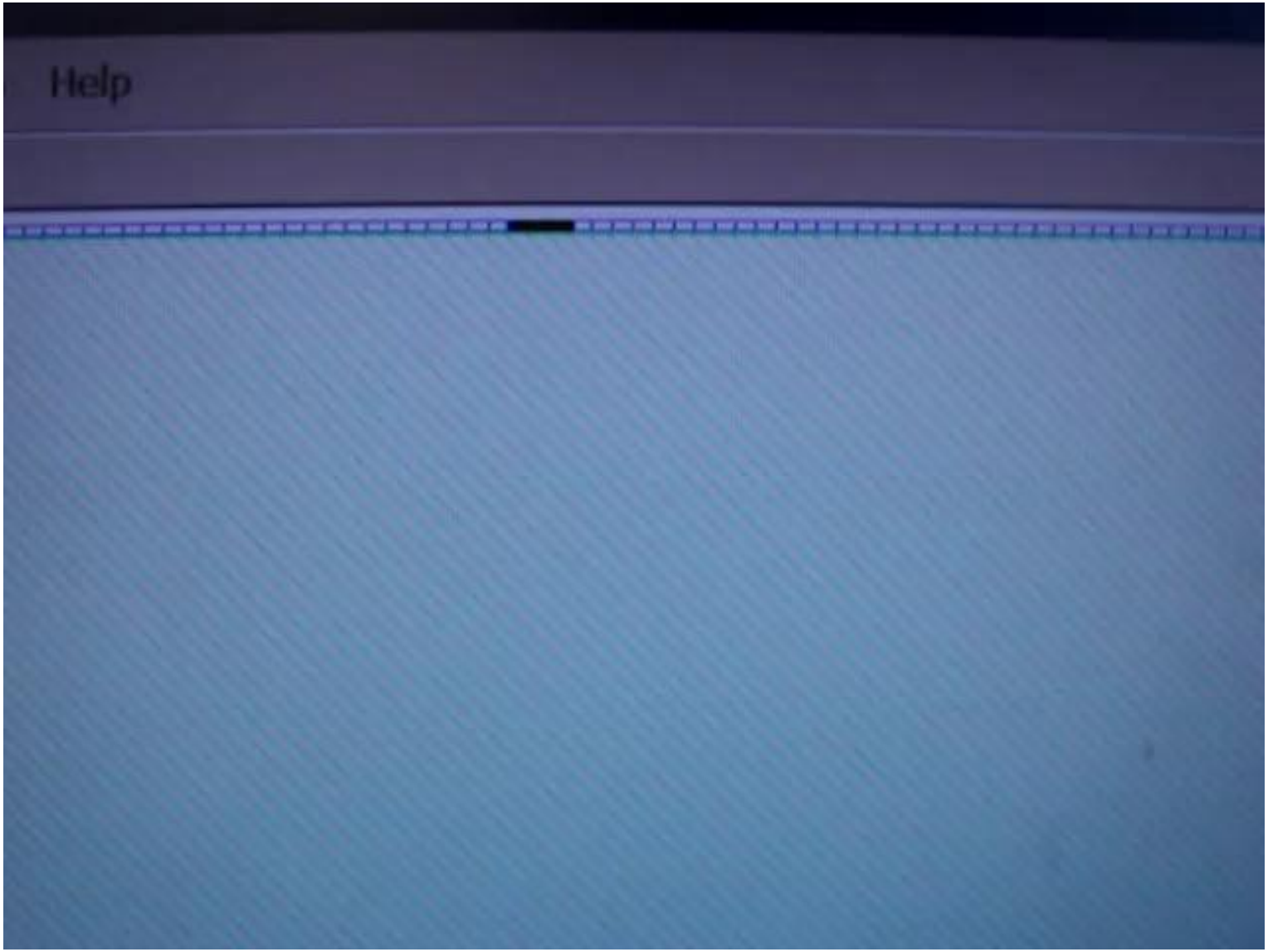








Ram Atomic Oxygen Attack at Crack Defect Site in Kapton H Polyimide (200,000 atoms entered)

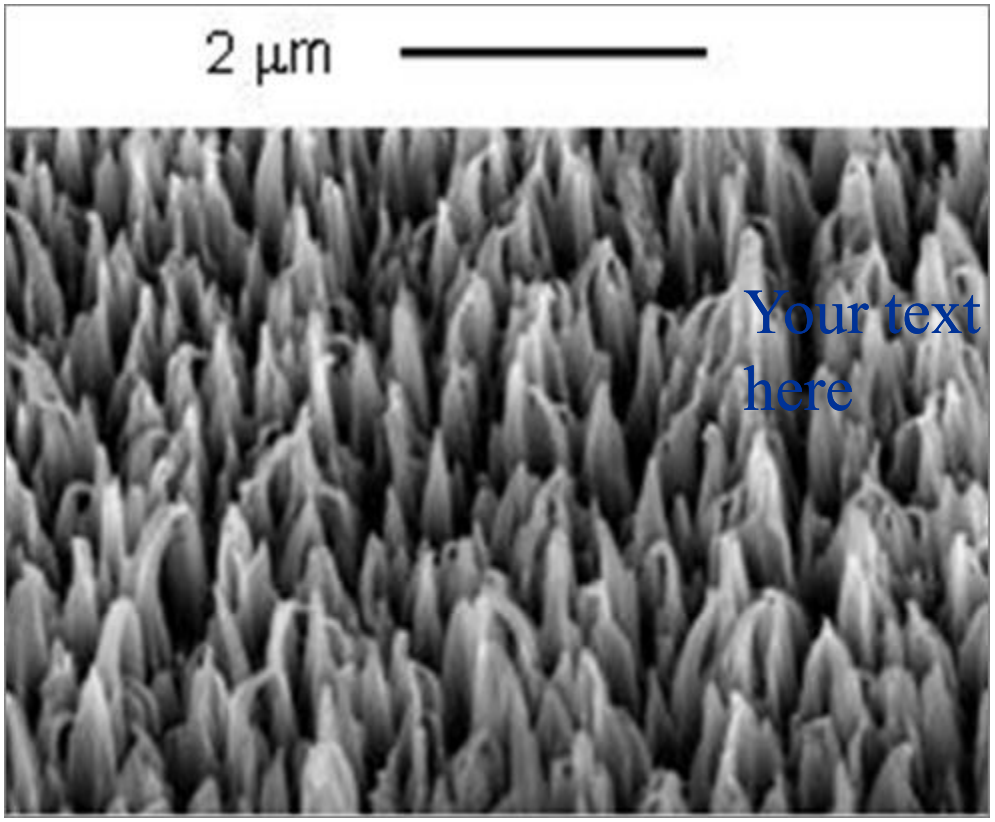


Interaction parameter	Value
Atomic oxygen initial impact reaction probability	0.062
Activation energy, E_A, in eV for energy dependent reaction probability	0.26
Atomic oxygen reaction probability dependence exponent upon angle of impact, n, where the reaction probability = $P_E \bullet (\cos\ q)^n$ where q is the angle between the arrival direction and the local surface normal and P_E is the energy dependent reaction probability at normal incidence	0.5
Probability of atomic oxygen recombination upon impact with protective coating	0.33
Probability of atomic oxygen recombination upon impact with polymer	0.3

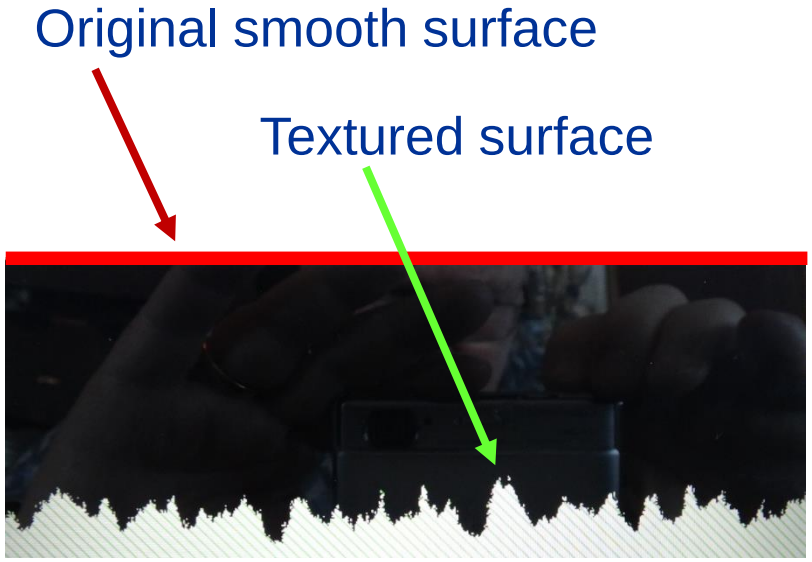
Fractional energy loss, *f,* upon impact with polymer	0.4
Fractional energy loss upon impact with protective coating	0.05
Degree of specularity as opposed to diffuse scattering of atomic oxygen upon non-reactive impact with protective coating where 1 = fully specular and 0 = fully diffuse scattering	0.2
Degree of specularity as opposed to diffuse scattering of atomic oxygen upon non-reactive impact with polymer where 1 = fully specular and 0 = fully diffuse scattering	0.5

Temperature for thermally accommodated atomic oxygen atoms, K	300
Limit of how many bounces the atomic oxygen atoms are allowed to make before an estimate of the probability of reaction is assigned	25
Thermally accommodated energy/actual atom energy for atoms assumed to be thermally accommodated	0.9
Initial atomic oxygen energy, eV	4.5
Thermospheric atomic oxygen temperature, K	1000
Atomic oxygen arrival plane relative to Earth for a Maxwell-Boltzmann atomic oxygen temperature distribution and an orbital inclination of 28.5^{o}	Horizontal

Monte Carlo Modeling Showing Development of Textured Surfaces

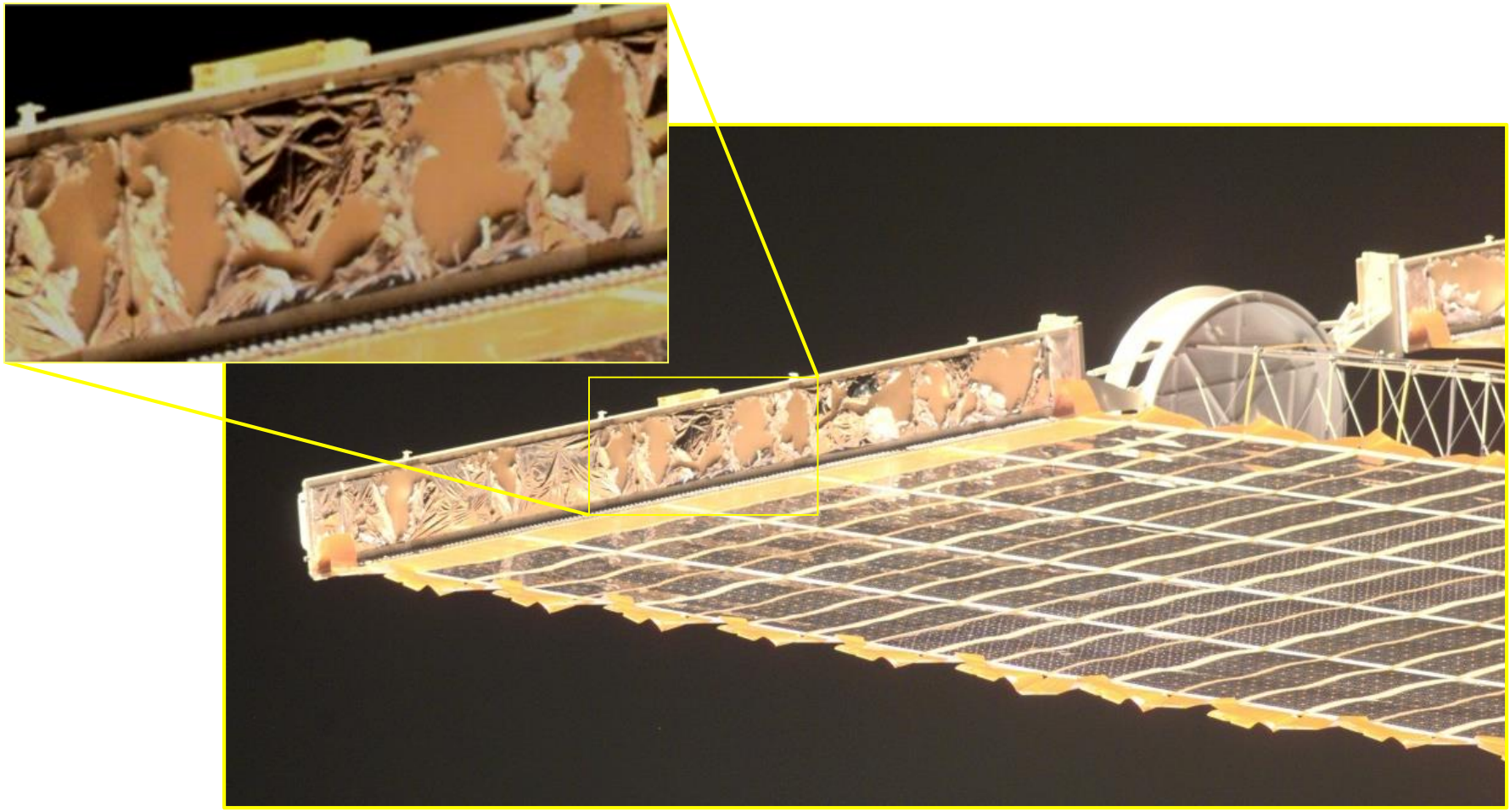


LDEF atomic oxygen textured surface

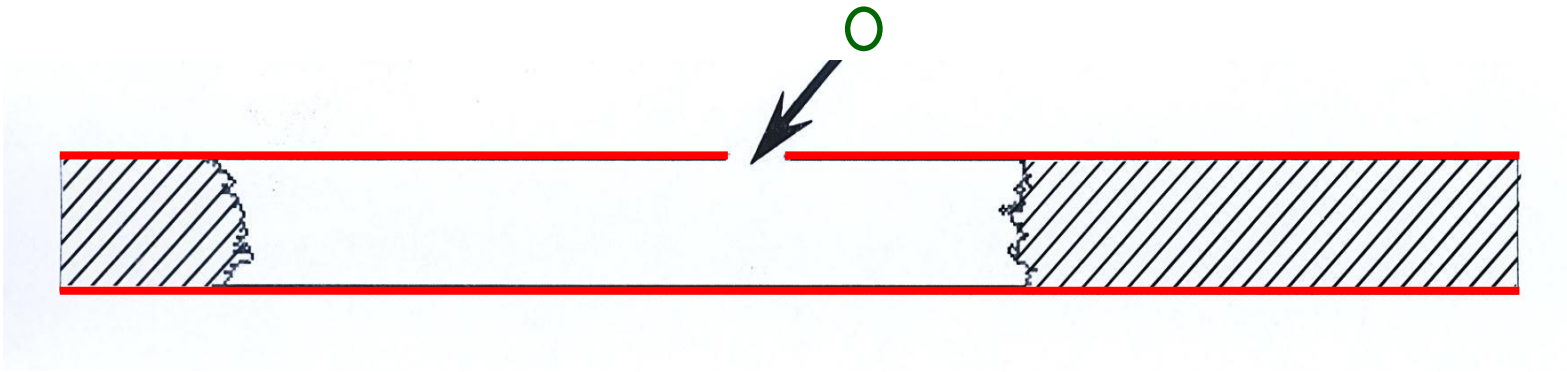


Monte Carlo model textured surface using 2 million simulated oxygen atoms

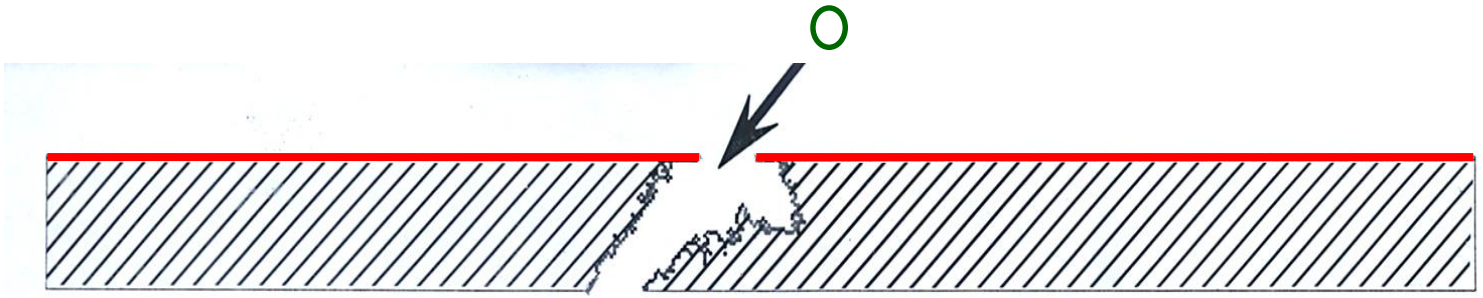
International Space Station Solar Array Blanket Box Covers After One Year In Orbit



Computational Predictions

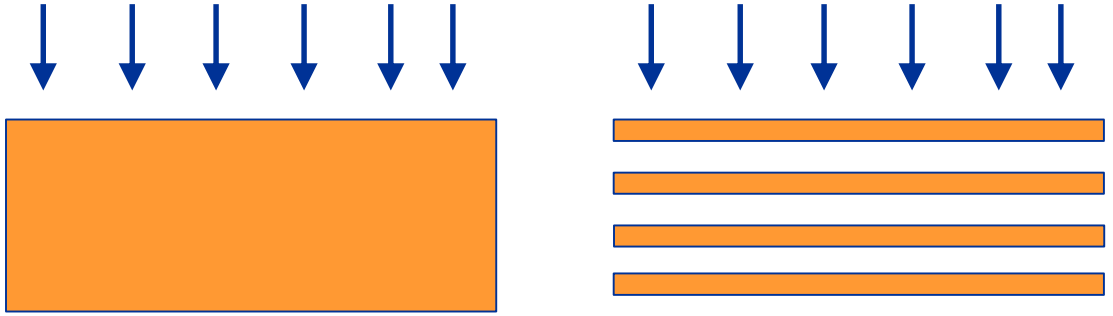


Double aluminized Kapton

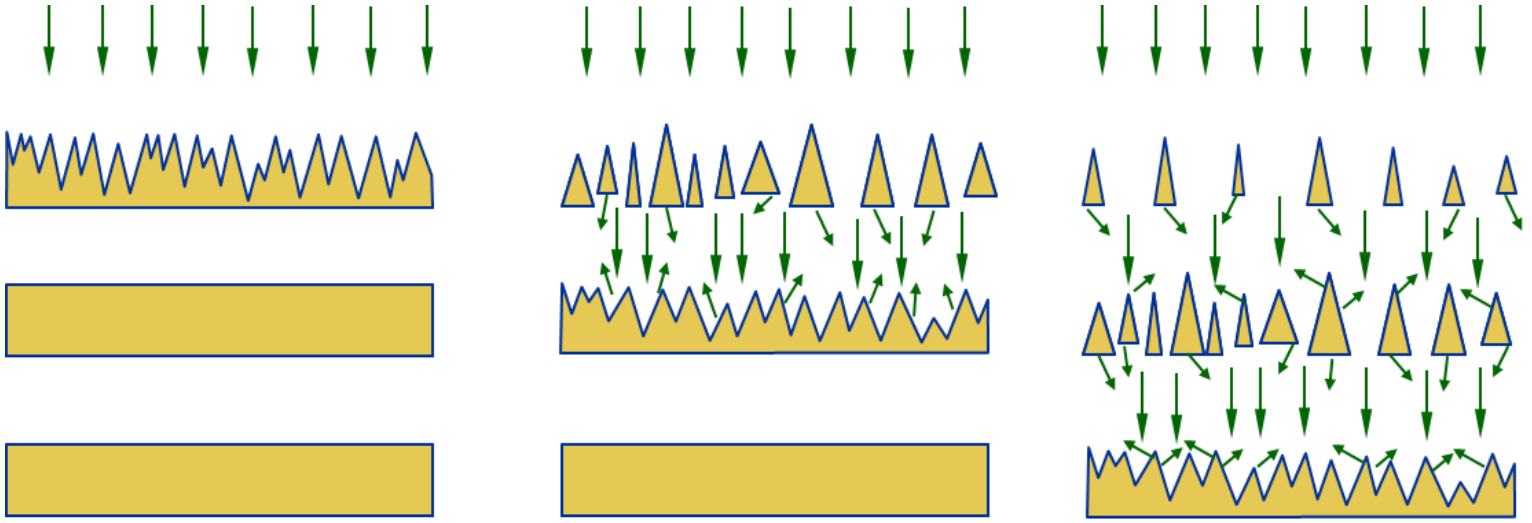


Single aluminized Kapton

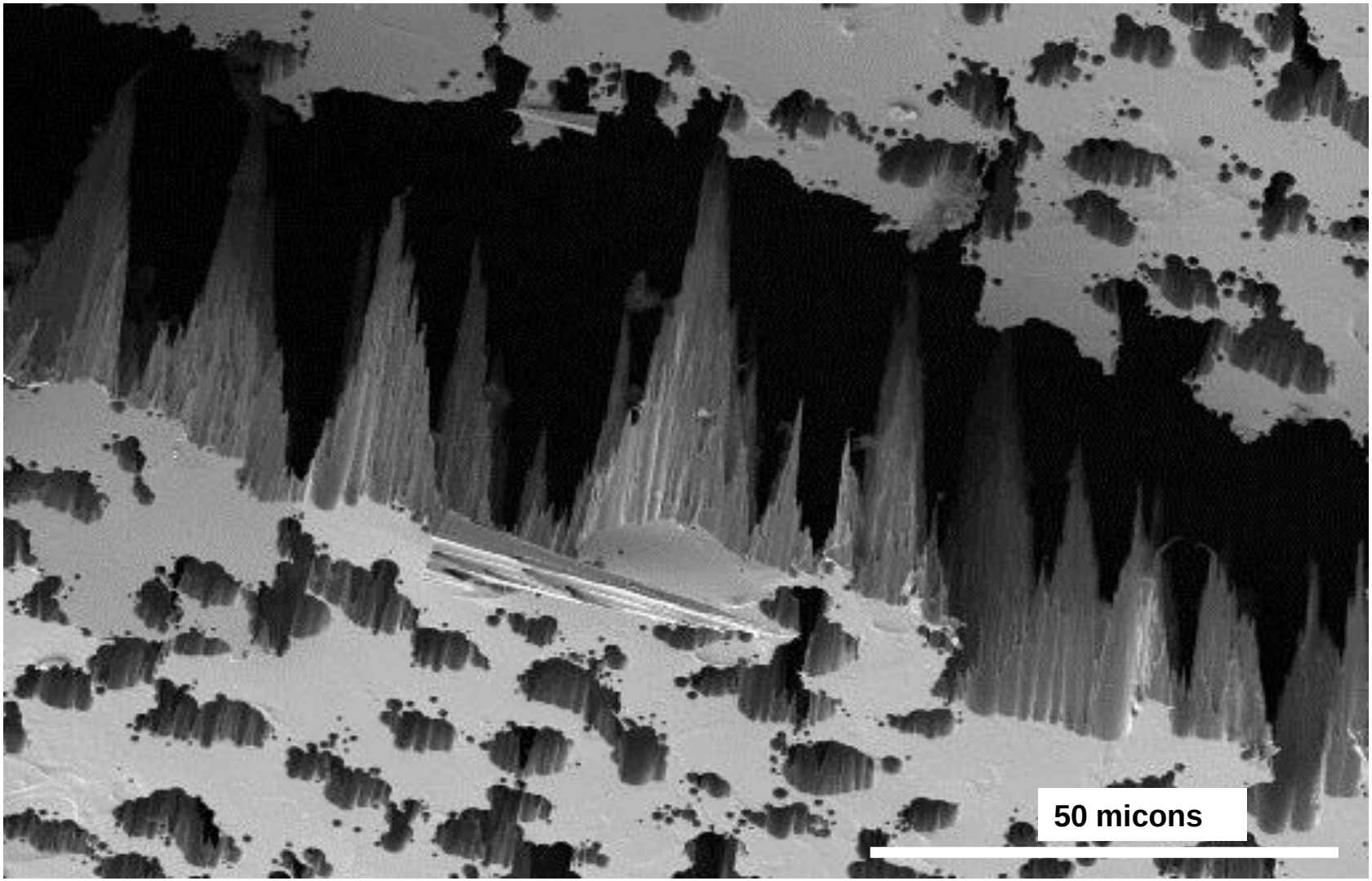
Atomic Oxygen Erosion of Single & Multiple Layer Polymer Films



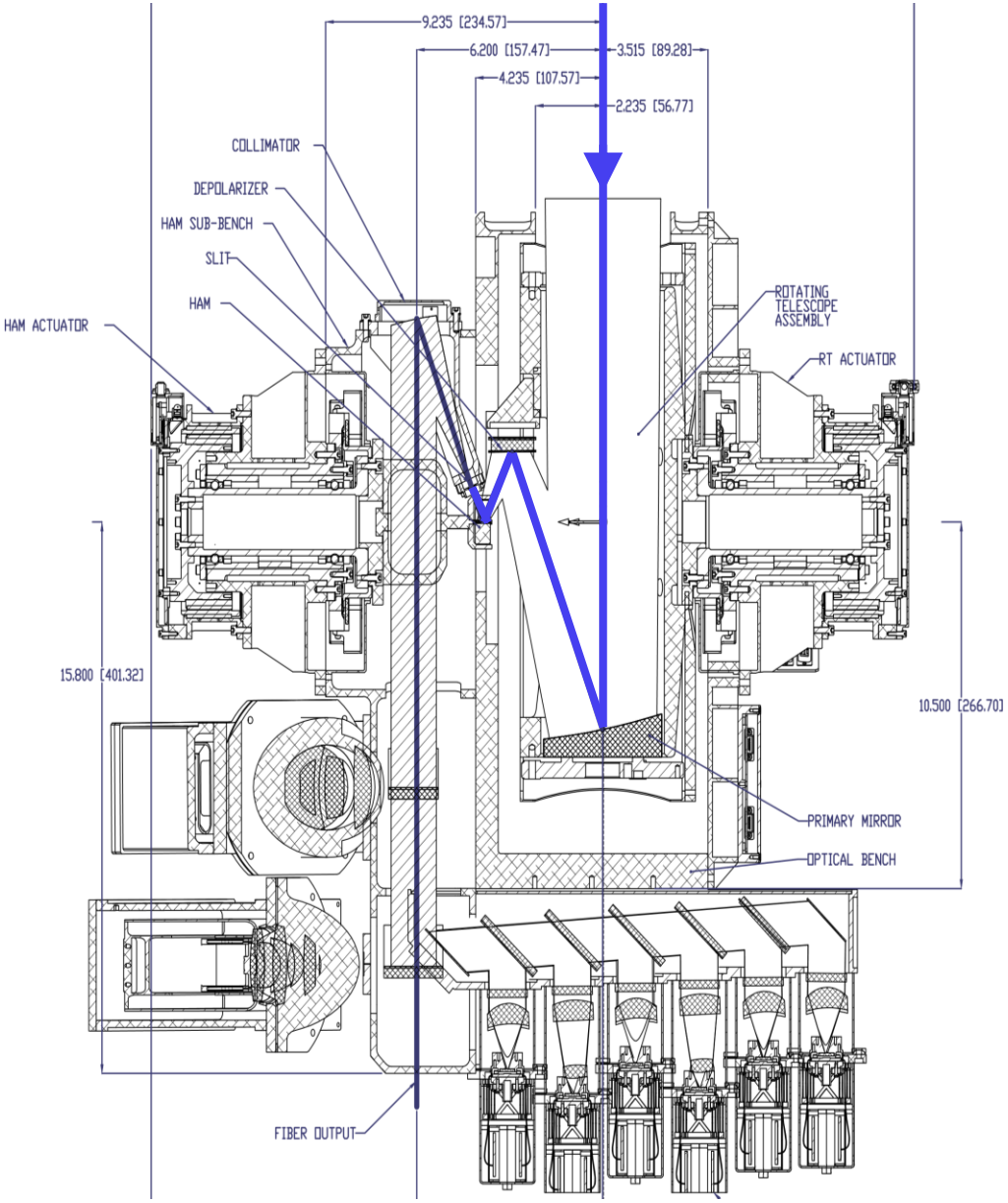
Erosion yield, $cm^3/atom$	3×10^{24}	3.25×10^{24}



Atomic Oxygen Erosion Thru a Thin Layer of Kapton H



Ocean Color Instrument



Conclusions

- Monte Carlo computational modeling of atomic oxygen interactions can be made to replicate observed in-space erosion of polymers.
- The interaction characteristics can be used to predict oxygen fluxes and potential interactions within telescopes and other low Earth orbital structures.
- Potential exists to determine durability issues representing a variety of polymers and structures.