Contribution ID: **72** Type: **Poster Presentation**

Reactive molecular dynamics simulations of the atomic oxygen impact on Poly(2,5-benzimidazole)

Tuesday, 4 July 2023 15:52 (1 minute)

The development of radiation shielding for spacecraft found in low Earth orbit (LEO) has been an ongoing campaign since 2001 [1, 2]. In the LEO range, various threats cause extensive degradation of spacecraft materials. Considering organic materials such as polymers have one threat that significantly affects them: atomic oxygen (AO). Atomic oxygen is formed via photo-disassociation of diatomic oxygen caused by solar radiation [3] with a flux of $\sim 10^{14} AO/cm\ s$ at energies of ˜5eV [4]. AO is the most abundant species found in the LEO environment and causes oxidative erosion of organic material. Testing the erosive nature of AO on a polymer proves difficult when considering the experimental apparatus required to replicate the AO impact on the material [4]. This difficulty is the availability of apparatus that can have AO as the bombardment species while performing the bombardment experiment at the required energy. In South Africa, very few nuclear accelerators have AO as the bombardment species, but these have energy constraints. A model is created for this investigation to perform AO bombardment on the poly(2,5-benzimidazole) (ABPBI) material and composite variations using reactive molecular dynamics (MD). The results from the MD simulations include mass loss, AO penetration depths, and temperature evolution with regards to AO impact on the material. In previous work, the authors performed AO bombardment on the polymer and its composite at the iThemba labs Gauteng. The intention of this work is to, through the reactive MD, compare changes to the samples as a result of varying energies.

1. de Groh, K.K., et al. MISSE PEACE polymers: an international space station environmental exposure experiment. in Proceedings of the AIAA Conference on International Space Station Utilization. 2001.
2. Kaminski, C., et al. MISSE PEACE Polymers-An International Space Station environmental exposure experiment. in 2001 Conference and Exhibit on International Space Station Utilization.
3. Dever, J., et al., Chapter 23 - Degradation of spacecraft materials, in Handbook of Environmental Degradation of Materials, M. Kutz, Editor. 2005, William Andrew Publishing: Norwich, NY. p. 465-501.
4. Kleiman, J., et al., Atomic oxygen beam sources: A critical overview. Materials in a Space Environment, 2003. 540: p. 313-324.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

Consent on use of personal information: Abstract Submission

Primary authors: ELLIS, Ernst (North-West University); SQUARE, Lynndle (North West University)

Presenter: ELLIS, Ernst (North-West University)

Session Classification: Poster Session 1

Track Classification: Track A - Physics of Condensed Matter and Materials