Electronic Supplementary Material (ESI) for RSC Advances.

Ferroelectric P(VDF-TrFE)/POSS Nanocomposite Films: Compatibility, Piezoelectricity, Energy Harvesting Performance, Mechanical and Atomic Oxygen Erosion

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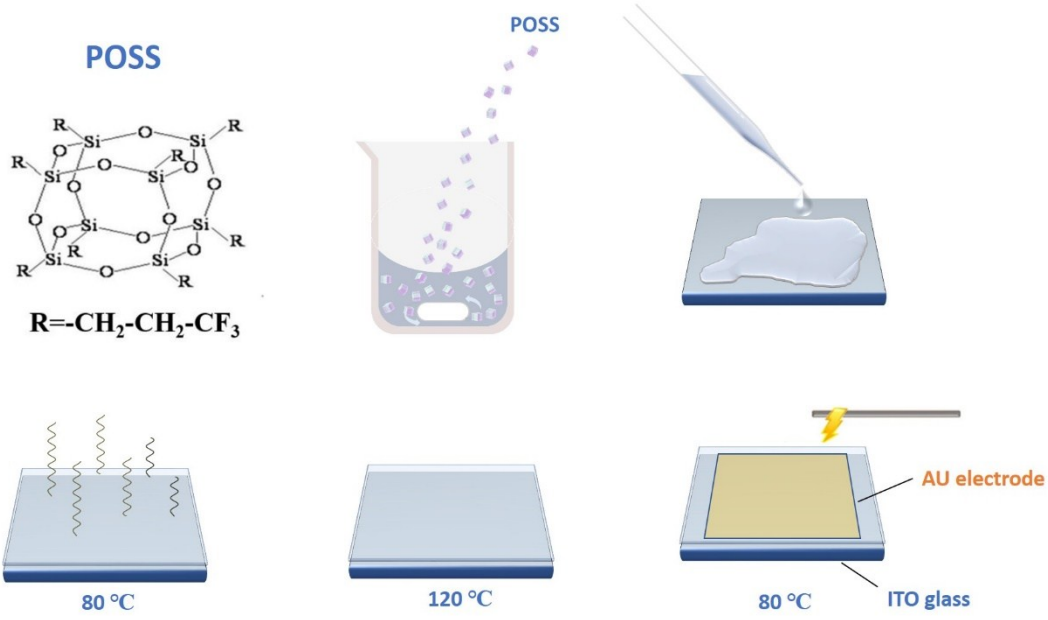

Fig.S1. The molecule structure of fluoropropyl POSS and the fabrication of piezoelectric composite

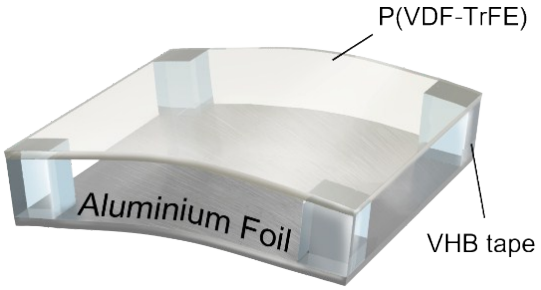

Fig.S2. The schematic diagram of triboelectric nanogenerator

The erosion yield and the atomic oxygen simulated number

The erosion yield and the atomic oxygen simulated number were the two primary parameters to determine in the simulation. The erosion yield describes the atomic oxygen resistance of the material and is related to the structure of the material. The erosion yield was calculated according to the following equation derived by NASA based on long term in-space flight simulation [1]:

$$\lambda = C_0 (V_\Sigma / V_r)^{C_{\Sigma/r}} (\rho)^{C_\rho} e^X \tag{1}$$

where λ was the erosion yield, which depended on the chemical structure and ingredient. C_o was proportionality constant. V_Σ was the sum of the volume of the atoms making up the polymer repeat unit based on their covalent radii. V_r was the actual volume of each repeat unit determined based on the chemical structure of the repeat unit and the molecular weight and density of the material. $C_{\Sigma/r}$ was constant for the ratio of total atomic volume in repeat unit. ρ was the density of polymer. C_ρ was constant for polymer density. The parameter X was calculated according to the following equation.

$$\begin{aligned} X = {} & (C_{C/t}N_C + C_{H/t}N_H + C_{sO/t}N_{sO} + C_{dO/t}N_{dO} + C_{N/t}N_N \\ & + C_{Cl/t}N_{Cl} + C_{F/t}N_F + C_{S/t}N_S) / N_t + (C_{O/C}N_O + C_{N/C}N_N \\ & + C_{F/C}N_F + C_{H/C}N_H + C_{Cl/C}N_{Cl} + C_{S/C}N_S) / N_C - K[(A)] / (1 - A) \end{aligned} \tag{2}$$

and

$$K = (1.80 \times 10^{-16}) F^{0.76} \tag{3}$$

The coefficient $C_{C/t}$, $C_{H/t}$, $C_{sO/t}$, $C_{dO/t}$, $C_{N/t}$, $C_{Cl/t}$, $C_{F/t}$, $C_{S/t}$, $C_{O/C}$, $C_{N/C}$, $C_{F/C}$, $C_{H/C}$, $C_{Cl/C}$,

$C_{S/C}$, and K were constants associated with the various terms relating to atom number in the repeat unit, physical density, composition of material, number of single or double bonded oxygen atoms, etc. N was number of related atoms. A was a mass fraction of ash in the polymer and F was atomic oxygen fluence[2, 3].

In order to simplify the simulation process, some appropriate corrections were made to the number of oxygen atoms and the size of the defect used in the simulation. The erosion yield of unprotected P(VDF-TrFE) was λ=2.56×10^{-21} mm^3/atom. Suppose a large defect with width of W_c = 50 μm and length of L_c=50 μm. The width is meshed to W = 500 elements during simulation, thus each element corresponds to the actual width of L = 0.1μm. Each atomic oxygen eroded one element during the simulation, so each simulated atomic oxygen represented real oxygen atoms with the number of L^3/λ. The number of oxygen atoms related to an atomic oxygen fluence of F could be calculated according to the following equation:

$$M = F \times L_c \times W_c \times C / (L^3 / \lambda) \quad (4)$$

where M was the number of oxygen atoms. F was atomic oxygen fluence, W_c and L_c were the width and length of large defect respectively. C equaled to the value of L_c/L. λ was the erosion yield.

The accumulated atomic oxygen fluence

The Low Earth orbit attributes ranging from 200 to 700 km in the ionosphere. The actual atomic oxygen flux is about 10^{11}~10^{15} atoms/cm^2 s. Assuming 3 years of an in-space test at an altitude of 500 km, the accumulated atomic oxygen fluence was 4.1×10^{20} atoms/cm^2, and atomic oxygen particles collided with a kinetic energy of 5 eV.

References

[1] Banks, B.A., Backus, J.A., Manno, M.V., Waters, D.L., Cameron, K.C. de Groh, K.K., Atomic oxygen erosion yield prediction for spacecraft polymers in low earth orbit, Proceedings of the ISMSE-11, 15 (2009) 18.

[2] Banks, B.A., Backus, J.A., Manno, M.V., Waters, D.L., Cameron, K.C. De Groh, K.K., Prediction of atomic oxygen erosion yield for spacecraft polymers, J Spacecraft Rockets, 48

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[3] Bank, B.A., de Groh, K.K. Backus, J.A., Atomic Oxygen Erosion Yield Predictive Tool for Spacecraft Polymers in Low Earth Orbit, (2008).