Ultrathin TMD space solar cells with multifunctional integrated device stack demonstrating high-specific power and space radiation resilience

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Abstract— Ultra-thin solar cells based on transition metal dichalcogenides (TMDs) offer several advantages over conventional solar technologies for space applications, including space radiation tolerance and high specific power. Due to the ultra-thin nature of the cells, they operate in a new regime and are vulnerable to very low energy radiation (<100 keV), especially protons. In this work, we simulate the radiation stability of WSe2based solar cells and designed a cell device stack to withstand low energy proton radiation that is present at high fluences levels in space. An integrated and multifunctional ultra-thin (<600 nm) space radiation shielding stack is designed to encapsulate and protect against radiation, while improving the anti-reflection and light absorption in the active layer, passivation, doping, and charge transport, and emissive radiative cooling. Our optimized design shows experimental results of minimal degradation after proton irradiation at realistic mission fluences, with nearly full recovery following operatingtemperature anneal process.

Keywords— transition metal dichalcogenides, solar cells, specific power, space radiation, radiation resilience, annealing

I. INTRODUCTION

Recent advances in inexpensive space launch technologies and reusable vehicles have made launch costs ~700 times cheaper than NASA's first rockets, opening up space access to technologies and missions that were previously deemed infeasible [1]. Rapid increases in space missions have placed new demands on the key enabling technology of solar power. Solar modules for space use have different requirements of their performance than those for terrestrial use: with high specific power (i.e. power-to-mass ratio) to maximize useful power output whilst minimizing launch mass; vacuum compatibility; temperature cycling; and critically, resilience against the harsh space radiation. Radiation in the space environment exhibits itself in the form of ionizing protons and electrons, atomic oxygen (in low Earth orbit), gamma, x-rays, ultraviolet radiation, and galactic cosmic rays.

Solar panels used for space missions are primarily made from now-mature III-V multi-junction cells. These cells are relatively vulnerable to damage from space radiation; to abate this, shielding cover glasses are typically applied to block all but the most energetic particles [2] - adding substantial amounts of nonfunctional mass to the mission. In recent years various novel materials have been used as energy harvesting layers in solar cells, such as organic components, perovskites, and more recently transition metal dichalcogenides (TMDs). These emerging materials, TMDs in particular, have absorptions that are higher than mature technologies, allowing for much thinner energy harvesting layers in the order of nanometers and thinner devices overall [3, 6]; this alters the radiation vulnerability profile of such ultrathin devices under space radiation [3, 4], and consequently affects the radiation energies and fluences they must be tested against for space qualification. Very low-energy proton radiation becomes critically important for demonstrating resilience of ultrathin solar cells in space environments.

II. TMD SOLAR CELLS

Compared to traditional cells, ultra-thin and flexible cells have several orders of magnitude higher specific power [3, 6]: enabling efficient optimization of launch system constraints. Apart from launch requirements, operation in space requires shielding from damaging radiation present in the space environment. Conventional cells achieve this by using thick, rigid, and bulky cover glasses (in the order of several hundreds of microns in present systems), which decreases their specific power further. With experimental demonstration and test results, we report on cover glassfree space radiation-hard ultrathin TMD solar cells.

Transition metal dichalcogenides (TMDs) possess excellent properties for space photovoltaics, including ultrahigh absorption coefficients, near-ideal band gaps, and self-passivated surfaces. Devices using TMDs as the energy material can take advantage of the higher absorption coefficient to use thinner layers of active material [6], reducing overall cell thickness. At these reduced thicknesses, high energy space radiation is able to pass through, potentially, without much damage; however particles at the extremely low energy end of the space radiation spectrum present a hazard: they are able to penetrate through the front layers, deposit energy and embed in the active layer, and cause damage. As traditional cells are much thicker and used a thick cover glass, the low energy space environment was of no concern as it was automatically blocked, however as devices push into the micron and nanometer regime where high energies are able to pass through the cell, the make-up and effects of this low energy portion of the spectrum becomes very important.

III. RADIATION HARDNESS

Our TMD cell stack is shown schematically in Fig. 1 [6]. Previous reports with perovskites, also in ultrathin film design, show that electron radiation causes substantially less damage than proton radiation [3], which was corroborated by simulations in CASINO (monte CArlo SImulation of electroN trajectory in sOlids) of our devices, leading to a focus on proton radiation tests. Incident proton radiation was simulated using the SRIM (Stopping and Range of Ions in Matter) software package. Cells with only a thin (~70 nm) passivation coating were vulnerable to ~22 keV protons, which is very low energy regime- an area where there is relatively poor or missing orbital and experimental data and protocols for space testing, and where the fluences are many orders of magnitude higher than at and above 100 keV (where data and protocols are present). The incident energy that the cells are vulnerable to can be tuned by designing an ultrathin shielding layer of SiO₂- MoO_x of less than 600 nm.



Fig. 1. Schematic of TMD solar cell with multifunctional ultra-thin SiO_2 - MoO_x (<600 nm) space radiation shielding layer designed to encapsulate and protect against radiation, while improving the anti-reflection and light absorption, passivation, doping, and charge transport, and radiative cooling.

Fig. 2 shows low energy protons and electrons (10 keV) being blocked from reaching the interfaces and energy layer in the cell (purple layer). **Fig. 4** shows higher energy particles at 100 keV, which penetrate to the TMD layer where they can potentially cause damage, however for these higher energies (>100 keV) the fluences present in space are several orders of magnitude lower.



Fig. 2. 10 keV radiation penetration simulation. Left panels show proton radiation, the blue dots in the upper panel indicate proton end positions after penetrating the material stack and stopping distances. Population statistics are shown in the histrogram beneath, and per-layer are summarized in the bar chart at the bottom. The layers of the stack are colour coded to Fig. 1, with the blue layer corresponding to SiO₂ shielding etc. The right panels show the electron penetration simulations. The upper plot shows where energy is deposited within the device stack, and the wireframe indicates stack layers. The lower plot shows a sub-set of individual electron trajectories, with colour scale representing the energy of the electron.

Fig. 2 shows that at very low energies the radiation fails to reach the active layer of the device stack and that the shielding layers successfully protected the device at these low energy but high fluence radiation present in space.

IV. MULTIFUNCTIONAL INTEGRATED RADIATION SHIELDING



Rear electrical contacts, photon recycling, heat spreader, and radiative cooling with deployable structural support

Fig. 3. Representational schematic of the space cell, showing multifunctional and integrated device stack.

We present a multifunctional layer design for space solar cells removing the need for heavy and thick cover glass (shown in **Fig. 3**). The shielding layer is multifunctional: protecting from space radiation while maximizing antireflection, light absorption in the active layer, passivation, doping, and charge transport, and emissive radiative cooling. Due to the differences in refractive index between the WSe₂ active layer, the MoO_x passivation-doping layer, and the SiO₂ shielding layer; the absorption in the WSe₂ layer is sensitive to the thicknesses of layers in the stack - allowing absorption to be optimized by varying the shielding thickness. By combining a shielding layer of 540 nm of SiO₂ on top of 50 nm of MoO_x passivation layer, we further reduced the total thickness of the effective shielding layer required. With this front side coating, the proton vulnerability energy of the cell was shifted away from the damaging low energy protons that are present in plentiful in the space environments. Within this shielding layer design, we optimized the light absorption in the active layer, and it increased from ~0.6 to ~0.8. The SiO₂ in the stack increases the bare cell front emissivity in the infrared region, giving an operating temperature that is well below the degradation temperature ranges of the materials in the cell stack. Emissivity can be further enhanced by structuring the SiO₂ or incorporating metallic oxide layers. The Au metallic back contact acts as a mirror, recycling photons back into the energy layer, and a heat spreader.



Fig. 4. 100 keV radiation simulation. Panels same as in Fig. 2.

Fig. 4 results show that both 100 keV electrons and protons can penetrate to the TMD layer with 600 nm of SiO_2 -MoOx shielding, however at and above 100 keV the fluences are several orders of magniture lower and the cell will survive this, showing that the vulnerability energy window and the resilence can be tuned with the design of the device layers.

V. EXPERIMENTAL RESULTS OF PROTON RADIATION TESTING

An ensemble of shielded and unshielded WSe₂ cells were irradiated with various proton energies and fluences and their performance was noted pre and post irradiation. One of the noteworthy results is after exposure to 88 keV protons at 10^{12} cm⁻¹ fluence, the power conversion efficiency of the unshielded cells were observed to decrease by 11.9% (**Fig. 5**). This small degradation is found to be reversible: thermal annealing at 90 °C was able to almost fully recover the cell (1% degradation) and lower temperature anneals up to 45% also show recovery. These temperatures are achievable during standard cell operation, allowing continuous or periodic in situ healing of the accumulated radiation damage and regaining of the cell's optoelectronic functionality. Analysing our results, we attribute the resilience and recovery of our TMD cells due to closeto-perfect and almost defect-free 2D layered structure, and specifically, carrier diffusion lengths that are two orders of magnitude larger than the absorber thicknesses in these TMD WSe₂ solar cells.



Fig. 5. Current density-voltage (J-V) characteristics of WSe₂ solar cells prior and after 88 keV proton radiation showing radiation resilience and recovery of unshielded cells, with 90°C anneal recovering the cell performance.

Fig. 5 shows that prior to irradiation, the device demonstrated a short-circuit current density (J_{SC}) of 25.84 mA cm⁻², an open-circuit voltage (V_{OC}) of 426 mV, a fill factor (FF) of 49.93%, and a power conversion efficiency (PCE) of 5.50%. Proton exposure led to a noticeable decrease in J_{SC} to 21.35 mA cm⁻², while V_{OC} increased slightly to 433 mV. FF improved modestly to 52.38%, but the overall PCE declined to 4.84%, corresponding to an 11.9% reduction in performance. This degradation was accompanied by an increase in series resistance (R_{S}) from 2.22 to 2.64 ohm·cm², and in shunt resistance (R_{SH}) from 53.58 to 90.41 ohm·cm².

Following a 1-hour anneal at 90 °C, the devices showed significant recovery. For the device in Fig. 5, FF increased substantially to 64.41%, while $V_{\rm OC}$ and $J_{\rm SC}$ slightly decreased to 417 mV 20.24 mA cm⁻². The PCE recovered to 5.44%, nearly matching the original preradiation value, with a net efficiency loss of just 1.0%. Concurrently, $R_{\rm S}$ decreased to 1.92 ohm·cm², and $R_{\rm SH}$ 241.88 ohm·cm², rose to indicating reduced recombination and enhanced charge transport. These results highlight the effectiveness of low temperature thermal annealing in mitigating radiation-induced performance degradation in ultrathin TMD solar cells. A full report on the shielded and unshielded devices post proton irradiation and anneal recovery will be presented in a follow up paper. The WSe₂ solar cells studied here show a power conversion efficiency of up to 5.5% under AM 1.5 illumination. This corresponds to a record specific power of 10.7 W g⁻¹ in TMD solar cells. Upon design optimization, TMD solar cells can achieve up to 25% power conversion efficiency [7], leading to unprecedented levels of power-per-mass of 48.8 W g⁻¹ (unshielded) and 38.7 W g⁻¹ (with multifunctional shielding).

VI. CONCLUSIONS

We report on space radiation tested ultra-thin WSe₂based solar cells for space applications, where the stack has been designed for multifunctionality of the layers to remove the unnecessary mass and maximize the specific power. Minimal degradation is observed after exposure to low-energy proton radiation. Annealing at operating temperatures is shown to recover most of the lost device performance after space radiation exposure, demonstrating in-situ repair of the devices, and suitability for space applications [5].

Contributions: O.T. and K.N. contributed equally as first authors. N.V. conceptualized the project and innovated the multifunctional device stack for ultrathin integrated space cell – encapsulate and space radiation shielding, anti-reflection, light absorption and enhancement, passivation, doping, and charge transport, and emissive radiative cooling. O.T. performed multi physics modelling and analyses, assisted by N.V. K.N. designed the TMD cells; and fabricated the devices, K.N. performed the J–V measurements and analysis of data, assisted by N.V. All authors contributed to the presentation and writing of the manuscript. N.V. supervised the work.

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