FROM NANOANTENNAS TO DEEP SPACE SATELLITES, ELECTRON EMISSION ENABLES EFFICIENT POWER GENERATION

Engineers at the Italian Institute of Technology (IIT) are using multiphysics analysis to illuminate ways electron emission can be used to improve power efficiency in extreme-environment technology and biomedical applications.

By **LEXI CARVER**

DEEP SPACE AND THE HUMAN BODY have something in common: the challenge of designing devices that can operate in them safely, reliably, and efficiently. For equipment used in aqueous conditions, severe temperatures, high pressure levels, and other extreme environments, stable and efficient power generation can be hard to come by. The search for better power efficiency in equipment such as deep-space satellites and medical devices has recently identified electron emission as a potential method of power generation.

Electron emission occurs when a metal surface or electrode is subjected to an electrostatic field, heat, or incoming light that causes electrons to escape the metal, often into a vacuum, so that they can be collected for usable electricity. The Italian Institute of Technology (IIT) and the European Space Agency (ESA) are collaborating to develop systems based on electron emission for solar power collection on deep-space satellites. Researchers at IIT are applying similar concepts to power nanoantennas for studying electrical signals in the brain. They use numerical analysis to study the behavior of emitted electrons and optimize their devices for best functionality and highest efficiency.

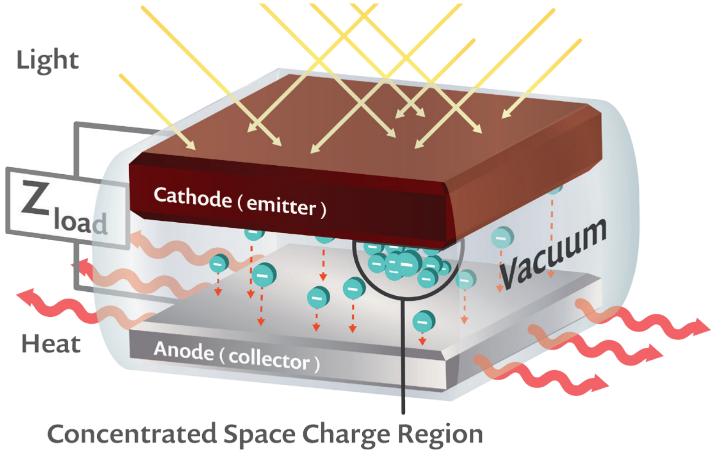

Figure 1. Schematic of a PETE. Electrons escape the cathode due to light (shone on the semiconductor) and heat (due to an electrical load). Space charge buildup occurs due to electrons getting "stuck" in the vacuum gap as they repel each other during travel to the anode.

» BETTER SOLAR POWER IS COMING TO SATELLITES

PHOTOVOLTAIC SYSTEMS CONVERT sunlight into electricity and are effective for solar panels on or near Earth, but are not very efficient for near-sun missions in deep space, where high temperatures destroy the efficiency of the photovoltaic conversion. Photon-enhanced thermionic emission (PETE) solar cells, first developed in 2010 at Stanford University, offer a promising alternative by combining photovoltaics with thermionic emission — the thermally-induced flow of charge that releases electrons from a heated semiconductor — to boost power generation.

A PETE cell (see Figure 1) comprises a vacuum chamber sandwiched between an anode and a cathode made of a semiconductor such as Gallium Arsenide. Incoming photons excite electrons in the valence band of the cathode into the conduction band, causing some electrons to be released into the vacuum gap and others to shift closer to the vacuum energy level of the semiconductor, readying them for easier escape by thermionic emission. Heating the cathode then causes more electrons to "boil" away into the vacuum gap. The freed electrons travel to the anode at the other end, where they create charge buildup that can be used for electrical power.

"Photon-enhanced thermionic emission takes advantage of the semiconductor structure of the cathode and the temperature difference between cathode and anode, transforming heat into electrical power," explained Pierfrancesco Zilio, a post-doctoral fellow at IIT. "Unlike standard photovoltaics, both the ultraviolet-visible and the infrared regions of the solar spectrum are exploited in the conversion, with the former promoting electrons to the conduction band of the semiconductor and the latter enabling their escape to the vacuum gap. "

However, the emitted electrons

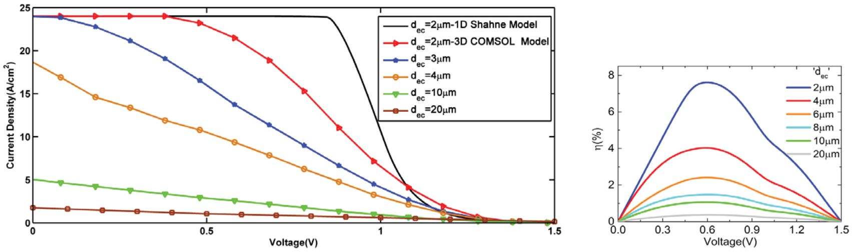

Figure 2. COMSOL® software results showing the current density at the anode (left) and power conversion efficiency (right), calculated for different distances between anode and cathode and different operating voltages.

repel each other, so some are deflected back to the cathode or get "stuck" in the middle of the vacuum gap. The latter case can create a space charge (SC) cloud that interferes with the further passage of electrons and strongly reduces the device efficiency.

» *SIMULATION LENDS A HAND*

ZILIO AND HIS COWORKERS Waseem Raja, a PhD student, and Remo Proietti, a senior researcher, worked with the ESA to investigate different PETE systems in order to maximize charge buildup at the anode and create a design robust enough to travel aboard deep-space satellites. They used COMSOL Multiphysics® software to study the PETE cell, creating several models to analyze possible designs and determine which ones would be most practical and efficient.

His team tracked the flow of electrons between the cathode and anode and studied the formation of the space charge cloud. They began with a model that calculated the electric fields at the cathode due to the photon impact and their absorption, then analyzed the effect this had on the electrons' ability to break free of the cathode surface.

"This allowed us to predict how the SC cloud formation would hinder electron accumulation at the anode, and therefore the final current output," Zilio said. "We calculated the barrier the electrons had to overcome in order to reach the anode, including the energy needed to free them from the cathode and the decelerating forces as they traveled due to the SC cloud."

Using numerical simulation they were able to test different layouts, changing the arrangement of the two electrodes in order to see which one resulted in the highest current output and efficiency (see Figure 2). "COMSOL allowed us to couple the space charge behavior to other physical effects involved, namely light absorption and carrier transport in the cathode."

To analyze electron emission and propagation in the vacuum chamber, they coupled a particle tracing model to the electrical and thermal model. "We determined the current density at the anode based on the electron trajectories and the electric potential," Zilio continued. "From there we calculated the net current output and the power conversion efficiency of the PETE cell for our chosen setup."

They also tested several strategies to minimize the space charge cloud. One concept used a cathode with a surface in the shape of a nanocone array, the rationale being that the sharp tip would result in a higher electric field and therefore more electrons emitted. Zilio modeled the electric fields and electron trajectories for a nanocone (see Figure 3), and evaluated the resulting current density at the anode.

Despite causing more electrons to be released from the cathode, the nanocone design was unable to overcome the SC cloud to increase the output current. So Zilio's team turned to a new tactic. "We added a positively-charged mesh gate in the vacuum gap to attract electrons as they are released and pull them across," he said. "This boosted electron extraction, strongly reducing the SC cloud between anode and cathode.

"Then we had to optimize the size of the holes and power used to charge the gate, so that we maintain the right compromise between efficiency, electron collection, and minimizing the number of electrons that get stuck to the gate."

They tested different pitch sizes (the distance between centers of adjacent holes) to see which gate configuration resulted in the highest current output at the anode. They also factored in the power fed to the gate, which affects the overall conversion efficiency. Figures 4 and 5 show results for different configurations, gate voltages, and pitch sizes.

From the simulations, the team chose a gate voltage, pitch size, and

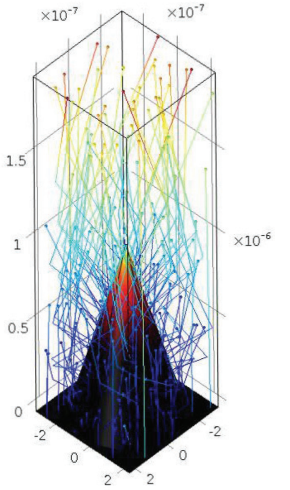

Figure 3. COMSOL results for the model of a nanocone. The plots show particle trajectories and velocity magnitude, as well as electric field norm throughout the cone surface.

> *"With the range of physics we needed to simulate, such as combining particle tracing with other behavior and including strongly nonlinear phenomena, COMSOL was a huge help.*
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> **— PIERFRANCESCO ZILIO, POST-DOCTORAL FELLOW, IIT**

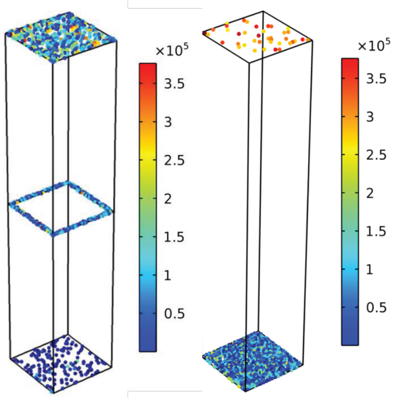


Figure 4. COMSOL results showing electron accumulation at the anode for cases with a gate (left) and without (right).

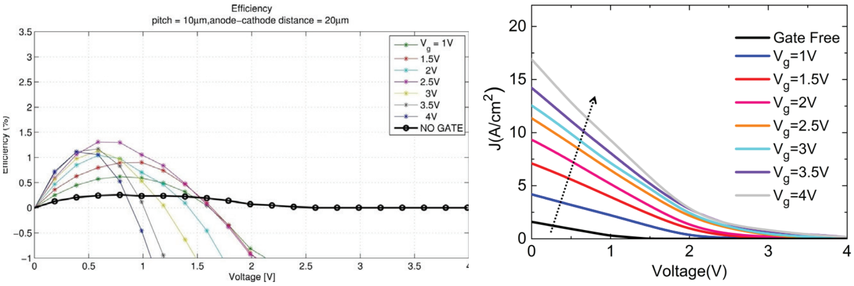


Figure 5. Simulation results show the power conversion efficiency for varying levels of voltage fed to the gate and a 20µm anode-cathode distance (left). The accumulated current density at the anode for different gate voltage levels and pitch sizes is shown at right.

anode-cathode distance to improve the efficiency of the design. Once they'd completed studies of the PETE cell, they used similar techniques to perform plasmonic simulations of nanoantennas for biomedical and neurological equipment.

» HOMING IN ON THE BRAIN

ZILIO ALSO USED ANALYSES IN COMSOL to investigate electron photoemission in nanoantennas, which are made of dielectric nanotubes coated with gold or silver (see Figure 6), when they are immersed in an aqueous environment representative of the human brain. These antennas will eventually be used to optically excite neurons, study electrical signals between them, and in medical treatment and diagnosis.

Submerging the antenna in a fluid environment lowers the work function, or the amount of energy required for an electron to be released from the metal. "This makes it easier for electrons to escape, but if the electron density around the antenna grows to a certain level, exponential ionization of the water molecules will occur and the antenna will no longer work," Zilio explained. Femtosecond laser pulses applied to the antenna cause plasmonic resonance that enhances the electric field at the surface of the metal, which increases the electrons' acceleration after emission.

Zilio's team coupled a simulation of the antenna's optical response to their model of electron emission and trajectories, and correlated the local field enhancement to the distribution of emitted electrons. His team then studied the "electrical hotspot," or the area with the highest electron density, and analyzed the catalytic reactions occurring based on collisions between water molecules and the emitted electrons. "The collision modeling functionality in COMSOL had everything we needed," he remarked. "I was able to simulate excitation, ionization, and elastic collisions all together."

The simulation (see Figure 7) revealed the electric field levels around the antenna and the hotspot, and predicted electron density and trajectories during release. After studying the antenna response as a function of height and laser power, the team to choose an operating range that would minimize risk of ionization and antenna failure.

» LOOKING AHEAD TO NEW TECHNOLOGY

AS THE IIT TEAM EMBARKED on the task of optimizing the performance of deep-space satellite devices and nanoantennas, the assistance lent by multiphysics analysis proved invaluable. "With the range of physics we needed to simulate, such as combining particle tracing with other behavior and including strongly nonlinear phenomena, COMSOL was a huge help," Zilio commented. From exploring the endless frontier of deep space to someday attempting to stimulate single neurons, engineers at IIT plan to continue using simulation to contribute to the development of technology in extreme environments. ◎

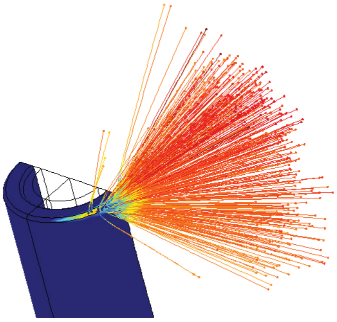


Figure 7. Particle trajectories as electrons are released from the metal.

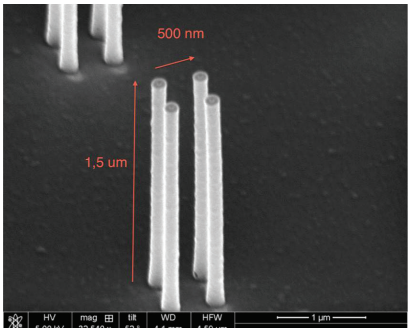
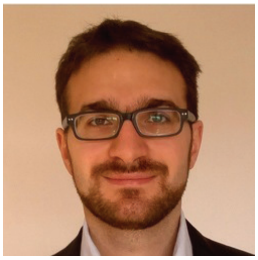


Figure 6. Close-up of gold nanotube antennas fabricated by secondary electron lithography. These antennas are able to produce strong plasmonic hotspots in the visible and near-infrared spectral ranges.



Pierfrancesco Zilio, post-doctoral fellow at IIT.