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HIGH-FIDELITY THREE-DIMENSIONAL SIMULATIONS OF THERMIONIC ENERGY CONVERTERS*

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Abstract

Thermionic energy converters (TEC) are a class of thermoelectric devices, which promise improvements to the efficiency and cost of both small- and large-scale electricity generation. A TEC is comprised of a narrowly-separated thermionic emitter and an anode. Simple structures are often space-charge limited as operating temperatures produce currents exceeding the Child-Langmuir limit. We present results from 3D simulations of these devices using the particle-in-cell code Warp, developed at Lawrence Berkeley National Lab. We demonstrate improvements to the Warp code permitting high fidelity simulations of complex device geometries. These improvements include modeling of non-conformal geometries using mesh refinement and cut-cells with a dielectric solver. We also consider self-consistent effects to model Schottky emission near the space-charge limit for arrays of shaped emitters. The efficiency of these devices is computed by modeling distinct loss channels, including kinetic losses, radiative losses, and dielectric charging. We demonstrate many of these features within an open-source, browser-based interface for running 3D electrostatic simulations with Warp, including design and analysis tools, as well as streamlined submission to HPC centers.

INTRODUCTION

Thermionic energy converters (TECs) generate electrical power from external heat sources using thermionic emission. By driving electrons across a narrow vacuum gap connected to an external load, electric power is created. For modest gap distances however, the thermionic current quickly exceeds the Child-Langmuir limit, reducing the peak achievable device power. To overcome space charge limitations an accelerating grid is used to compensate the negative potential generated by the beam space charge. The efficiency of such a device is theoretically limited only by the difference in temperature between the hot emitter and cold collector. However, the presence of a grid, along with realistic material properties of the device, serve to reduce their efficiency. Sophisticated simulations are needed to properly capture these dynamics.

Previous efforts to address these needs led to the development of an efficiency model and self-consistent simulation procedure for evaluating TEC designs [1]. In this paper we provide a brief review of this model and its implementation using the Warp particle-in-cell framework [2]. We then illustrate the value of this model in optimizing devices using a simple case study in grid placement and transparency. Lastly, we discuss the improvements being made to the electrostatic solver within the Warp to further improve vacuum nano-electronic device modeling.

EFFICIENCY MODEL

Energy conversion in a TEC is limited by a set of discrete loss channels, including kinetic, thermal, radiative, and resistive losses. Proper evaluation necessitates the tracking and quantification of each loss channel. For the Warp simulations discussed in these studies, we've adopted a model that is well-established in literature [3] and has been applied in recent experimental studies [4].

The model identifies four main loss mechanism of power from the TEC system: power carried by electrons leaving the emitter P_{ec}, net radiative power from the emitter P_{R}, conductive heat loss in the attached circuit P_{ew}, and finally power lost from holding the voltage on the grid P_{grid}. We note that the simulations assume periodic boundaries, and so the current and corresponding power quantities are normalized by area. The conversion efficiency of the device is the ratio of the net electrical power generated divided by the net thermal power exhausted. If the electrical power that is generated from circuit load is P_{load}, the efficiency η is:

$$\eta = \frac{P_{\mathrm{load}} - P_{\mathrm{grid}}}{P_{\mathrm{ec}} + P_{\mathrm{R}} + P_{\mathrm{ew}}} \,. \tag{1}$$

The net power transmitted from emitter to collector is:

$$P_{\mathrm{ec}} = J_{\mathrm{e}}\left(\phi_{\mathrm{e}} + 2k_{\mathrm{B}}T_{\mathrm{e}}\right) - J_{\mathrm{c}}\left(\phi_{\mathrm{e}} + 2k_{\mathrm{B}}T_{\mathrm{c}}\right) \,. \tag{2}$$

Here, J_{e}, the current leaving the emitter, is known exactly from the simulation. The second term accounts for return current back to the emitter. The emitter and collector work functions are ϕ_{e} and ϕ_{c}. The collector is assumed to be held at a low temperature ($T_{\mathrm{c}} < 500°$ K), thus we analytically compute the return current J_{c}.

The radiative heat loss is based on an analytic calculation for infinite parallel plates with some shielding from the grid. This is calculated as:

$$P_{\mathrm{R}} = \epsilon\sigma_{\mathrm{sb}}\left(T_{\mathrm{e}}^4 - T_{\mathrm{c}}^4\right) \,, \tag{3}$$

where ϵ is an effective emissivity, σ_{sb} is the Stefan-Boltzmann constant, and T_{e} and T_{c} are the emitter and collector temperature respectively.

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The power dissipated from the circuit is calculated as:

$$P_{\mathrm{ew}} = 0.5\left(\frac{L}{\rho_{\mathrm{ew}}}(T_{\mathrm{em}} - T_{\mathrm{env}})^2 - \rho_{\mathrm{ew}}(J_{\mathrm{ec}} - \mathrm{t}J_c)^2\right), \qquad (4)$$

where J_{ec} is the current density from the emitter that reaches the collector, known exactly from the simulation. The resistivities ρ_{ew} and ρ_{cw} account for the emitter and collector side wiring respectively and are calculated as a function of temperature.

The power lost in the gate is calculated based on the grid voltage V_{grid}, the current density striking the grid J_{grid} and the estimated return current, taking into account the geometric transparency, t, of the grid:

$$P_{\mathrm{grid}} = V_{\mathrm{grid}}\left(J_{\mathrm{grid}} + (1 - \mathrm{t})J_c\right). \qquad (5)$$

Finally, the power generated by the TEC is simply calculated from net current at the collector J_{ec} and the load voltage V_{load}:

$$P_{\mathrm{load}} = J_{\mathrm{ec}}V_{\mathrm{load}}. \qquad (6)$$

Simulation Procedure

The efficiency model described by Eq. (1) is only valid for steady-state operation. Reaching steady-state requires that the transient dynamics dissipate prior to collecting electron current information. In particular, fluctuations in current near the space-charge limit along with corresponding exter-nal circuit feedback must first subside.

In a TEC, current drawn through a load prompts a subsequent decrease in the effective voltage across the gap. An external circuit model permits these time-varying adjustments to maintain an accurate, self-consistent current value as the device reaches steady-state. We have implemented such a model, using Python hooks into Warp to adjust the gap voltage concurrently with the simulation. These adjustments can be made with arbitrary stride, meaning that fast fluctuations driven by noise in the simulation may be period-averaged to obtain an accurate correction. The resistance of the load is pre-computed based on the temperature and work functions of the emitter and collector and estimates for circuit material properties. Further details on this implementation can be found in [1].

We have developed a general procedure for verifying steady-state operation along with segregating measurements from this initial background. The procedure divides a simulation into four phases. The first two phases consist of initial emission of background electrons, during which current and circuit fluctuations are allowed to subside. Next, uniquely tagged "measurement" particles are emitted, from which statistics are collected for computing efficiencies. During the final phase of the simulation, background particles are re-emitted and any remaining "measurement" particles are allowed to complete their trajectories. This procedure is controlled using Python hooks into the Warp simulation, enabling user-defined feedback and consistency checks. Figure 1 provides a graphical schematic of this procedure.

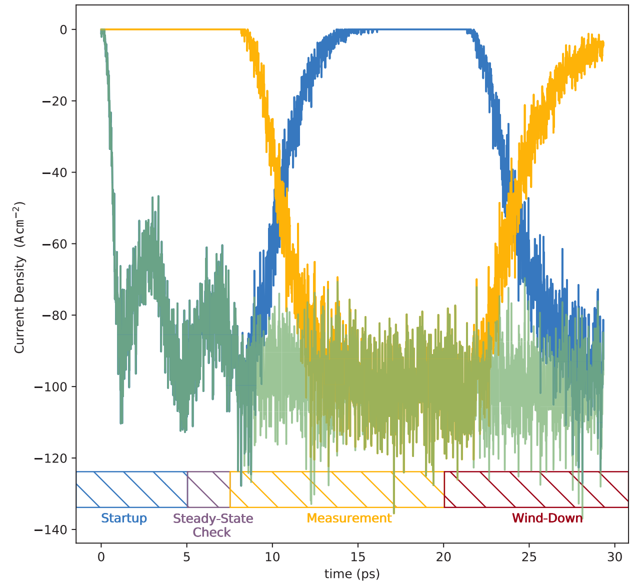

Figure 1: The four phase measurement scheme for validating steady-state and registering measurement particles [1].

GRID POSITION STUDIES

The need for self-consistent modeling and a comprehensive efficiency model can be seen even when considering a single design parameter. In this case, we consider the role of grid position in a TEC and its influence on device efficiency. We maintain fixed cathode and anode configuration, and vary the position of a grid with fixed geometry. In this case, the grid consists of a 4x4 rectangular lattice of struts, each 5 nm in width and depth. Simulations are performed with varying cathode temperature and grid voltage, and the grid transparency is computed for each run. In each case, grid transparency is only weakly coupled to temperature and to voltage. Figure 2 depicts this dependance on voltage.

We conclude that grid transparency scales roughly linearly with position along the z-axis, peaking when the grid is roughly 80% of the way across the gap. This behavior can be explained by the relative change in transverse momentum of the electrons due to the change in grid position. When the grid is near the cathode, a considerable fraction of the electrons' momentum is in the transverse plane, thereby increasing the likelihood of impact with the grid. When the grid is moved closer to the anode, the transparency increases due to the effective reduction in transverse momentum. Figure 3 illustrates this relationship.

Implementing the efficiency model quickly identifies a preferred operating point amongst otherwise indistinct conditions. Figure 4 reveals that the efficiency peaks for small voltages before rapidly declining. The reason for this is well understood from the transparency dynamics and the grid loss relationship described by Eq. (5). While the transparency remains relatively unchanged with increasing voltage, the power lost on the grid increases linearly with voltage. Thus, the optimal voltage is the smallest value to permit the full thermionic current to cross the gap.

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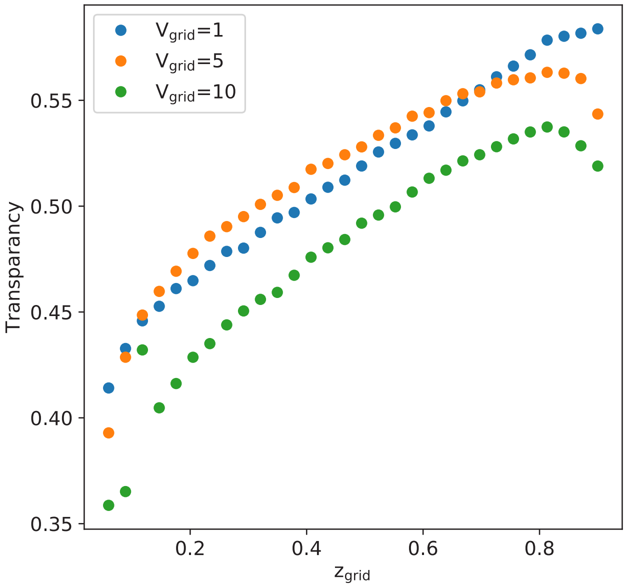

Figure 2: Grid transparency varies only weakly with grid voltage for fixed device geometry.

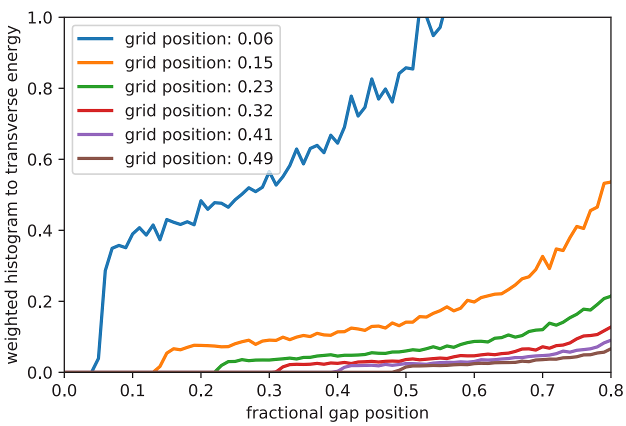

Figure 3: Electron transverse momenta are much larger at the point of grid crossing for grid positions nearer to the cathode. Grid transparency is subsequently reduced.

IMPROVEMENTS TO THE WARP CODE

Highly resolved, self-consistent simulations of emitted electrons and their interactions with the device geometry are required to properly implement these models. To this end, we employ the Warp particle-in-cell framework, currently in development at Lawrence Berkeley National Laboratory. Warp is a three-dimensional, time-dependent, multi-species PIC framework, which includes a a flexible array of solvers for obtaining electrostatic self-fields from Poisson's equations, or full electromagnetic fields from Maxwell's equations [2]. Most TECs operate in a low energy regime for which an electrostatic description will suffice, so we limit our consideration to the electrostatic components of the code.

Here we discuss recent work with the Warp code to improve the modeling of similar classes of vacuum nanoelectronic devices. Although the Warp code contains myriad

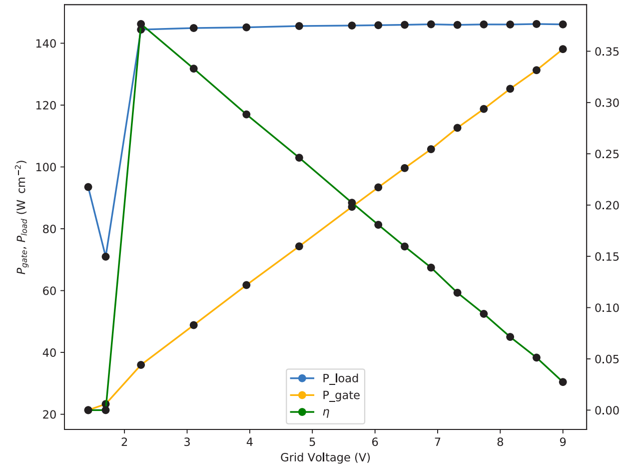

Figure 4: Efficiency, η, as a function of grid voltage, including kinetic losses and other terms in the model. The efficiency quickly peaks for small voltages, as the current crossing the gap and thus the load power P_{load} saturates. Additional applied voltage serves only to increase losses on the gate, as represented by the increasing P_{gate} curve.

features, further development is required to improve operation in the space-charge limited regime, along with the inclusion of three-dimensional internal dielectric structures.

Self-consistent Emission Models

In order to reach peak efficiencies, TECs must be operated with a large temperature differential. This is usually accomplished through increasing the emitter temperature, thus generating very high peak currents. The combination of high currents with small device size means that operation is oftentimes space-charge-limited. Therefore, proper device modeling requires an emission model which takes into account beam self-fields as well as external applied fields, even when operating at high temperatures. To this end, we have validated the Schottky emission model in Warp for thermionic emission with large applied fields in the space-charge limit.

For a cathode at temperature T, with work function ϕ_{e}, the current density j_{T} is given by

$$j_{\text{T}} = AT^2 e^{-(\phi_{\text{e}}-\Delta\phi)/k_{\text{B}}T} \,, \tag{7}$$

where k_{B} is Boltzmann constant, and $\Delta\phi$ is the effective change in work function of the material, resulting from an external electric field E according to

$$\Delta W = \sqrt{\frac{e^3 E}{4\pi\epsilon_0}} \,. \tag{8}$$

This simple model is effective at describing emission behavior in the presence of modest space-charge fields and applied fields up to $\sim 10^8$ V/m. Warp simulations of a simple diode with varying applied field and cathode temperature show good agreement with this model, as can be seen in Fig. 5. Furthermore, the space-charge forces of the beam are

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properly accounted for as well, and emission is limited by the Child-Langmuir law in these cases, as shown in Fig. 6.

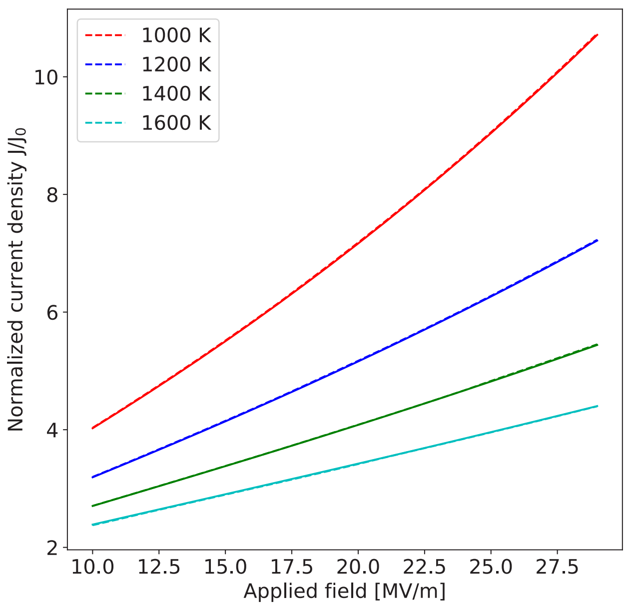

Figure 5: Normalized current density is plotted as a function of applied field on the cathode surface for several cathode temperatures. The simulated current density in Warp shows excellent agreement with the analytic prediction from Schottky emission theory

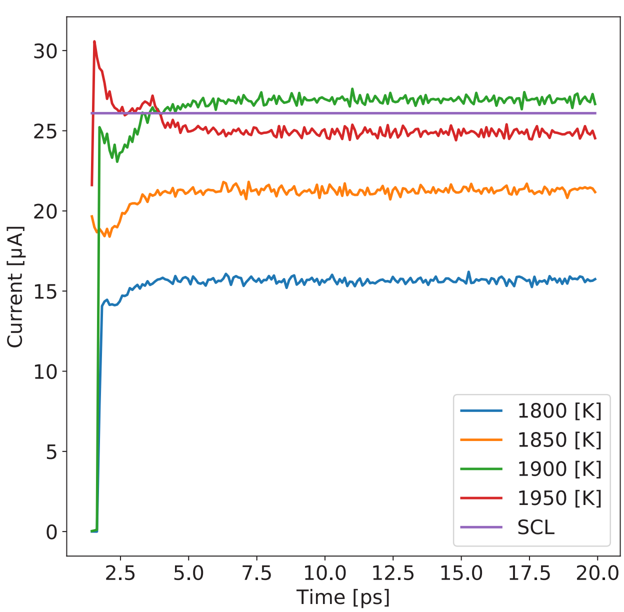

Figure 6: As the space-charge limit is approached with increasing temperature, the simulated emission shows small fluctuations in time before settling to the expected value.

Dielectric Solver

For the parameter regime under consideration, we use Warp's electrostatic multi-grid solver to obtain solutions to Poisson's equation. The advantage of this solver for TEC modeling is the ability to incorporate complex boundary conditions using the Shortley-Weller method to obtain subgrid-resolution representations during the solve [5]. As a result, a higher order stencil can be used to obtain accurate representations of the fields near surfaces with minimal additional computational cost. Internal dielectrics may be specified, but the solver has historically only supported 2D geometries.

We have extended this multi-grid dielectric solver to work in 3D, and enabled parallel execution of the solver using Warp's standard MPI decomposition scheme. We have performed benchmarks against analytically solvable systems, for instance a dielectric sphere placed between a cathode and anode held at fixed potential. Figure 7 shows a slice of the solution to the electrostatic potential, along with a lineout comparing the result to theory.

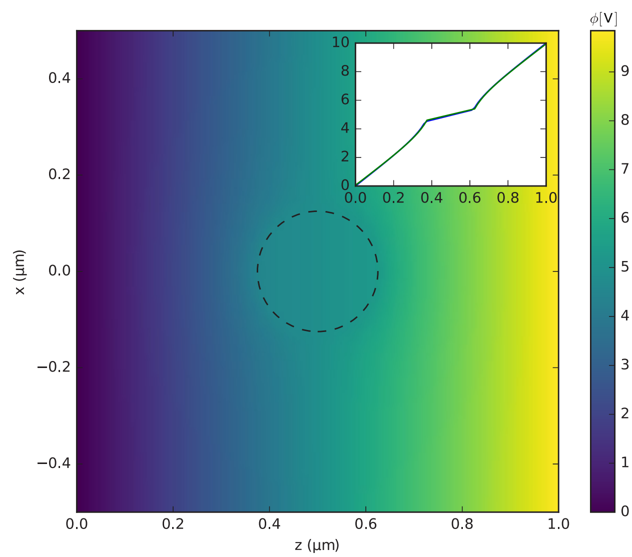

Figure 7: A 2D slice of the simulated potential between two parallel plates with a dielectric sphere placed in-between. Inset, a central lineout shows good agreement with theory.

In addition to extending the available geometries, we have also added the capability of dielectric structures to capture charged particles on their surface. Due to the limited charge mobility, dielectric structures in a TEC may slowly become charged from electron collisions, leading to the development of local field perturbations along the structure's surface. These fields may alter particle trajectories, changing the steady-state operation of the system. Warp has been outfitted with the capability to tag captured particles on dielectric surfaces. These particles remain fixed at the location of their intersection with the surface, and contribute to the surrounding electrostatic potential. Figure 8 shows the effective charging of a slab of dielectric resulting from the impacts of incoming electrons.

CONCLUSION

We have developed self-consistent tools using the Warp code to model thermionic energy converters. We then implemented and tested a well-established efficiency model for

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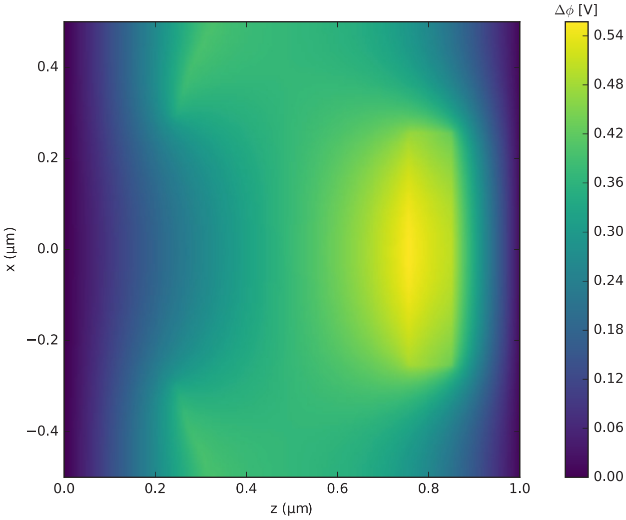

Figure 8: The dielectric particle implementation permits the buildup of surface charge due to impacts by electrons.

computing the individual loss channels and overall efficiency of TEC devices. An external circuit model was also included, which adjusts the potential at the collector to provide realistic feedback. These models have proven effective in identifying design guidelines for basic TEC structures. Further improvements have been made to Warp to support internal dielectrics, which are necessary for supporting structures in realistic devices, and may alter steady state operation.

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