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Simulation Studies of Low Work Function Hollow Cathode Emitter Materials

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Abstract

Low-work function materials are of special interest to plasma thrusters for space applications, solar cells in renewable energy and other electronic devices due to their thermionic emission characteristics. This paper deals with low-work function materials, modelling and simulation aspects to demonstrate the features of thermionic emission. The material properties of low work function are obtained from experimental values reported in the literature. The thermionic emission characteristics are addressed by modelling the hollow cathode emitter as a hot cathode in a vacuum diode using a COMSOL Multiphysics environment. The emitted electrons give rise to space charge, which helps in identifying the potential drop across the diode. The potential drop is compared with the Langmuir-Fry model. Furthermore, simulations are performed to obtain the saturation currents for the insert materials. Cerium hexaboride has shown higher saturation current in comparison to Lanthanum hexaboride, Tantalum, Tungsten and Molybdenum. Though Lanthanum hexaboride is widely used as a hollow cathode emitter, the results encourage the consideration of Cerium hexaboride as a promising alternative.

Major Findings: *The planar diode simulation studies helped rank emitter materials through developed electric potential and current saturation studies. Cerium hexaboride, Lanthanum hexaboride and Tantalum are recommended emitter materials.*

Keywords: *Emitter Insert, Hollow Cathode, Thermionic Emission, Vacuum Diode, Work function*

1.0 Introduction

Electric propulsion offers higher specific impulses due to high-velocity ions at the exit plume for a low propellant flow rate. Hollow cathodes are key elements in electric propulsion systems for spacecraft, crucial for long-duration and efficient space missions. They generate electrons in Hall thrusters and ion engines to ionise the propellant gas, primarily xenon, to create the plasma necessary for thrust. Additionally, it neutralises the positively charged ion plume, which prevents electrical charge buildup on the spacecraft[1].

A typical hollow cathode comprises a cylindrical refractory tube that consists of a cathode tube, heater, emitter, keeper electrode and an orifice plate. The cathode tube is the main structure of a hollow cathode that houses low-work function emitter inserts, such as Lanthanum hexaboride (LaB_6), which is responsible for the generation of electrons during operation. The heater is a coil, wound around the emitter, which increases the insert surface temperature required for thermionic emission. The keeper is an electrode, placed near the cathode, which is used for ignition and maintenance of

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Table 1. Hollow cathode materials

Sl No.	Material	Description
1	Tungsten	Tungsten was one of the earliest materials to be used in a hollow cathode due to its high melting point and excellent electron emission properties[3,4].
2	Molybdenum	With similar properties to tungsten, Molybdenum can withstand high temperatures due to a high melting point[4].
3	Barium oxide	With a low work function of 1.0 eV, it is capable of efficient electron emission at lower temperatures[4,5].
4	Lanthanum hexaboride	LaB_6 has a work function of about 2.7 eV making it extremely efficient to operate at low temperatures while offering a high electron emission efficiency[3].
5	Cerium hexaboride	This is another advanced material with excellent emission properties and a work function of 2.5 eV used in high-performance hollow cathodes[6].
6	Iridium	It has a work function of 5.3 eV, which is relatively high but it compensates with its durability and longevity.
7	Others	Various alloys, such as tungsten-rhenium (W-Re) are used in hollow cathodes to enhance the mechanical properties and electron emission efficiency.

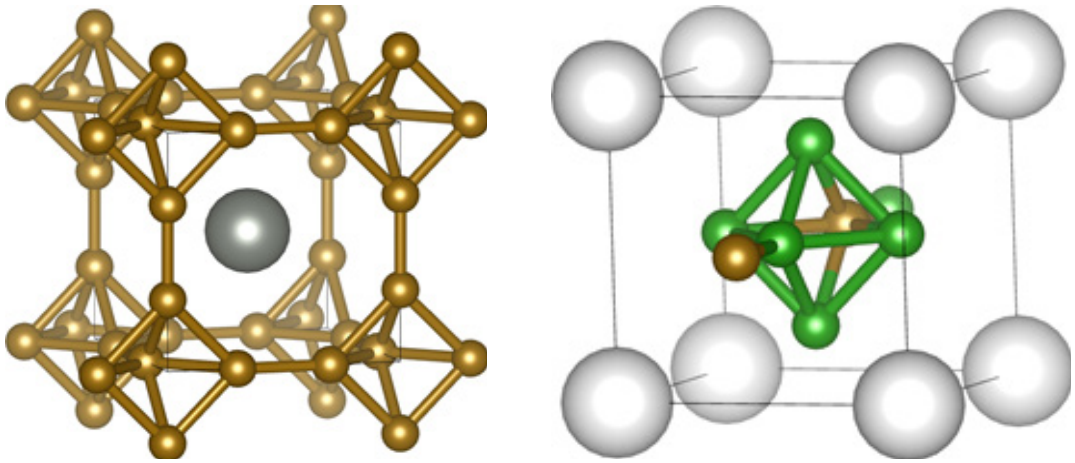


Figure 1. Lattice configuration of CeB_6 (left) and LaB6 (right) visualised using VESTA software.

the discharge[1,2]. Popular hollow cathode emitter materials and their attributes are listed in Table 1.

The work function of the cathode material is crucial for optimising the performance of a hollow cathode. This can be obtained by experimental methods such as photoelectric measurements, ultraviolet photoelectron spectroscopy and thermionic emission. Computational methods are also emerging. An accurate value of the work function of the material helps in determining the overall efficiency and electron emission properties of the cathode material.

Hollow cathodes impregnated with Calcium, Barium and Aluminum oxides are known to have a work function lower than 2 eV. However, due to their affinity towards cathode poisoning, materials like the LaB_6 are preferred. Cathode poisoning refers to the phenomenon of increased work function and the corresponding decrease in electron emission efficiency[1]. As indicated by Warner[7], Lanthanum

hexaboride performs better than Cerium hexaboride due to this reason. However, it is also important to consider other advantages of Cerium hexaboride, such as a work function of 2.5 eV that makes it a promising alternative[8].

It is possible to obtain the work function of the materials from the first principles utilising Density Functional Theory (DFT)[9]. It maps the electron structure of the system including molecules, surfaces and crystals. It uses electron density as a variable to simplify the computations against the quantum mechanical approach. DFT utilises supporting libraries for pseudopotentials[10] and material libraries[11] for lattice parameters and coordinates. These can help to predict improvements in material properties such as work function to recommend property enhancements using thin films or doping. Figure 1 illustrates a VESTA visualization of the LaB_6 and CeB_6 lattices used in such DFT calculations.

Electric thrusters face a wide array of challenges to qualify for enhanced thrust, efficiency, high specific impulse, long operational lifetimes, economical design, reduced channel erosion and resolved instabilities such as breathing instabilities. Hence, simulating and computationally verifying the performance of the thruster is essential for innovative design, analysis and optimisation before fabrication and experimental adaptation.

To simulate electric thrusters, multiphysics environments are appropriate. Before building the complex configuration of ionisation of propellant gas within the thruster and hollow cathode, it is important to simulate individual subsystems. It has to incorporate plasma discharge of propellant gases[12], magnetic circuit optimisation[13] and electrons from the cathode to demonstrate thrust generation. In the case of the operation of a hollow cathode, it is important to demonstrate thermionic emission. Hence, a planar diode is considered in this study, whose modelling aspects of space charge distribution and saturation currents are of special interest to this present work. The COMSOL Multiphysics environment is used in this study and discussed in Sections 2 and 3.

2.0 Materials and Methods

The work function is the minimum energy required to remove an electron from the surface of a material. The thermionic emission of a material is dependent on the work, given by the Richardson-Dushman Equation (1):

$$J = AT^2 \exp\left(\frac{-\Phi}{kT}\right) \quad (1)$$

Here, J represents current density, A is the Richardson constant, T is the absolute temperature of the metal, Φ work function and k is the Boltzmann constant. To increase the generation of electrons, materials should have a lower work function and high melting point, making them more effective for hollow cathode applications as they can resist higher temperatures while also emitting electrons. In addition, the important equations used to perform the simulations include Equations (2)-(7) for electrostatic computation and bidirectional coupled particle tracing.

$$\nabla . D = \rho_v \quad (2)$$

$$E = -\nabla V \quad (3)$$

$$\frac{\partial \rho_s}{\partial t} = \sum_{i=1}^{N} \frac{f_{rel,j} e Z_j}{meshvol} \quad \text{, where} \quad \bar{\rho_s} \quad \text{is given by} \quad (4)$$

$$\bar{\rho_s} = \frac{\bar{\rho}_{s,prev} + \frac{iter}{\beta}\bar{\rho_s}}{2} \quad \text{for iter} \leq \beta \text{ Otherwise, it is represented as,} \quad (5)$$

$$\bar{\rho_s} = \left(\sum_{j=1}^{i} w_j\right)^{-1} \left(\left(\sum_{j=1}^{i-1} w_j\right)\bar{\rho}_{s,prev} + w_i \bar{\rho_s}\right),$$

where i = iter -β+1 (6)

$$F_t = \frac{d(m_p v)}{dt} \quad (7)$$

Equation (2) is a Gauss law variant using D to define the electric field displacement, while Equation (3) represents the electric field E as the gradient of the electric potential V. Equation (7) is the kinetic adaptation to represent change in momentum. In addition, COMSOL uses Equation (4)-(6) on its backend to numerically compute the iterative results on its constructed mesh nodes[14].

2.1 Thermionic Emission in a Planar Diode

The hollow cathodes used in electric propulsion have a wide array of research interests. The work addresses the

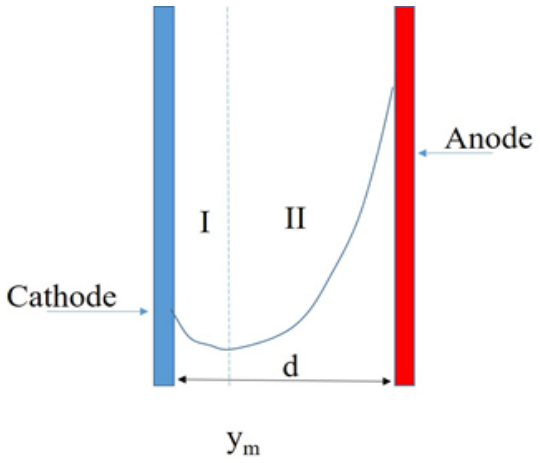


Figure 2. Illustration of a planar diode.

thermionic emission of the cathode insert, responsible for ionising the propellant using thermionic emission. Though the cathode contains other elements such as the refractory tube, orifice and heater, the insert material quantifies the performance of the cathode[1]. The insert material has evolved over the years with the shift being shaped by wide considerationson cathode life, operating temperature, cathode's affinity to poisoning and work function[1]. In this study, the thermionic emission is described as a functional parameter for the different insert materials used in hollow cathodes by treating them as hot cathodes.

The materials were simulated in COMSOL Multiphysics using a benchmark model of a planeparallel vacuum diode illustrated in Figure 2. The planar diode comprises two parallel electrodes, where the cathode is maintained at a constant temperature hosting the insert. The region between the electrodes gives rise to a space charge density due to the emitted current on thermal excitation. The diode's potential barrier restricts the free flow of the emission current, transmitting only the high-energy electrons.

A COMSOL benchmark build of the vacuum diode is used in the study. The multiphysics integration of electrostatics and charged particle tracing modules computes the particle field interaction. The simulation is performed using a vacuum boundary condition in a bidirectionally coupled particle tracing study. The study is simulated for a benchmark time of 0.1 microseconds. This offers the ability to extrapolate thermionic emission characteristics by computing the transmitted current. A theoretical reference from the Langmuir-Fry model is used to compare the COMSOL output.

Table 2. Input parameters of the vacuum diode with initial conditions for LaB_6 emission

Sl No.	Description	Variable	Values
1	Electrode Side Length	Rc	0.01m
2	Electrode Distance	D	0.001m
3	Anode Voltage	Va	100V
4	Cathode Temperature	Tc	1000K
5	Cathode Work Function	Phim	2.5V
6	Richardson Constant	A0	1.1 x 10^6 A/ (m^2K^2)
7	Particle Positions	N	100
8	Particles in velocity space per release position	Novel	50
9	Anode Current Density, reference	Jaref	-2535.6 A/m^2
10	Anode current, reference	Iref	-0.25356A
11	Location of the electric potential minimum, reference	Yref	1.1412 x 10^{-5}m
12	Electric Potential minimum, reference	Vref	-0.17937V

Hence, the electric potential developed within the diode is computed, while incorporating bidirectional coupled particle field interactions. The simulation output of the electric potential was compared with the analytical solutions derived from the Langmuir-Fry Model[15,16]. The diode adheres to the benchmarked values, whose initial conditions are specified in the parameters in Table 2.

2.2 Cathode Material Evaluation

The simulation is performed by varying the work function of the material and the excitation temperature. Based on the model's ability to reach convergence, the temperature has been varied across three temperature regimes listed in Table 3, testing important hollow cathode materials. The low-temperature regime is used for materials with low work function, while the high-temperature regime is reserved for high-work function materials.

2.3 Saturation Current Evaluation

As suggested by Hemenway *et al*[17], the current between applied potential increases until it saturates, where increasing the potential has no further effect on the net current. This observation can be found in the Current vs Voltage plots (I-V characteristics) listed in Section 3.2, where the saturated current forms a visible plateau upon increasing the potential difference[18]. Here the materials have been plotted in their respective temperature regimes, except Tantalum, which was previously simulated at 2000K is now plotted in a 2400K temperature regime.

2.4 Case Study on Lanthanum Hexaboride

A detailed case study is conductive for Lanthanum hexaboride, which is widely acknowledged as the most versatile insert in electric propulsion. It is due to high electron emission efficiency and low work function, making it an ideal thermionic emitter. In addition, its thermal stability, high melting point and long lifetime allow it to operate at extreme temperatures for durations that are far longer than the thruster life.

3.0 Results and Discussions

3.1 Cathode Material Simulations

The simulation studies were performed for the hollow cathode materials. The experimental work functions were obtained through literature and temperature regimes were assigned to simulate them as a hot cathode. The values in Table 3 were assigned alongside the initial conditions for the parameters listed in Table 2. The corresponding electric potential developed in the planar diode was inferred. A reference plot was generated to compare the simulation results with the analytical solution derived from the Langmuir-Fry model. Outputs featuring a minima as the lowest potential are shown in Figures 3 to 5. Hollow cathode keeper temperatures are set close to the emitting temperatures of the insert. The temperature regimes for keeper temperatures are selected to compare the performance of emitters that belong to the same category. For instance, Cerium hexaboride (Work function 2.5 eV) and Lanthanum hexaboride (Work function 2.66 eV) possess comparable emission temperatures. However, Molybdenum and Tungsten require higher keeper temperature regimes.

The derived values feature is used to quantify addition diode characteristics from the above plot groups. The position and magnitude of the minima (Potential minimum and its location) from the above graphs are

Table 3. Work function and allocated temperature regime for the simulations

Sl No.	Compound	Symbol	Temperature (K)	Work function (eV)
1	Cerium hexaboride[8]	CeB_6	1500	2.5
2	Lanthanum hexaboride[1]	LaB_6	1500	2.66
3	Tantalum[1]	Ta	2400	4.15
4	Tungsten[1]	W	2500	4.5
5	Molybdenum[1]	Mo	2500	4.85

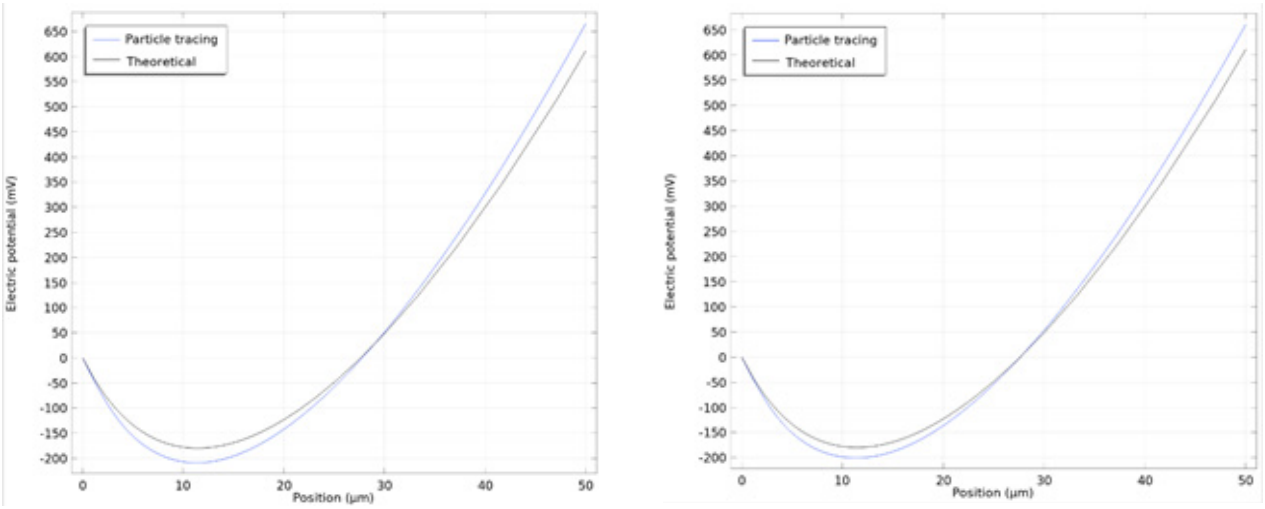


Figure 3. Electric potential across the planar diode for Cerium hexaboride (left) and Lanthanum hexaboride (right) at the 1500 K regime.

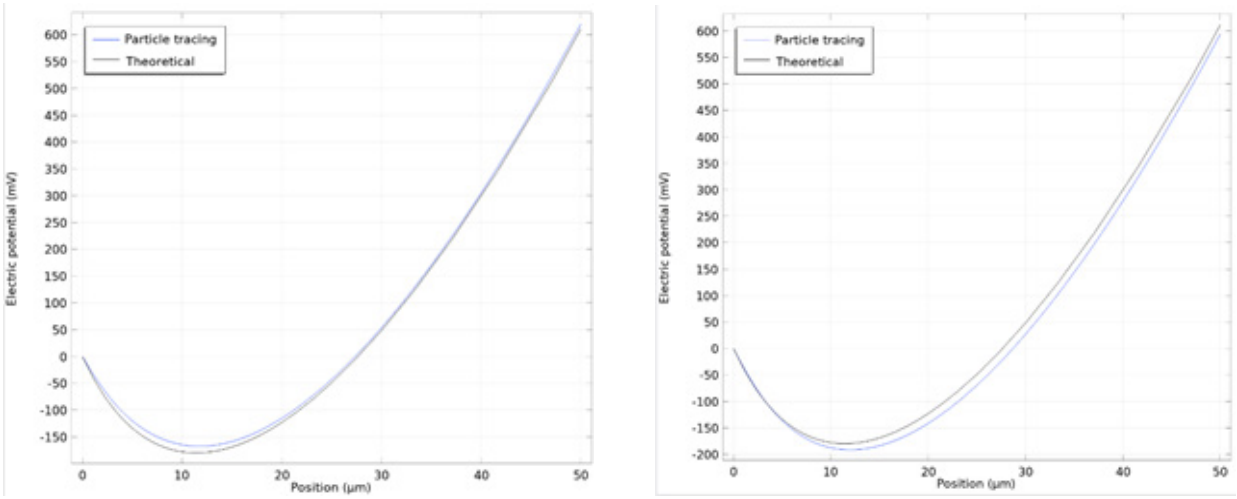


Figure 4. The electric potential across the planar diode for Molybdenum (left) and Tungsten (right) at the 2500 K temperature regime.

Table 4. Diode Characteristics for inserts

Sl No.	Compound	Potential Minimum (mV)	Location of Potential Minimum (μm)	Saturation Current (A)
1	Cerium hexaboride	-208.47	11.285	0.263
2	Lanthanum hexaboride	-199.97	11.285	0.264
3	Tantalum	-173.98	11.285	0.269
4	Tungsten	-191.06	11.788	0.269
5	Molybdenum	-167.2	11.788	0.27

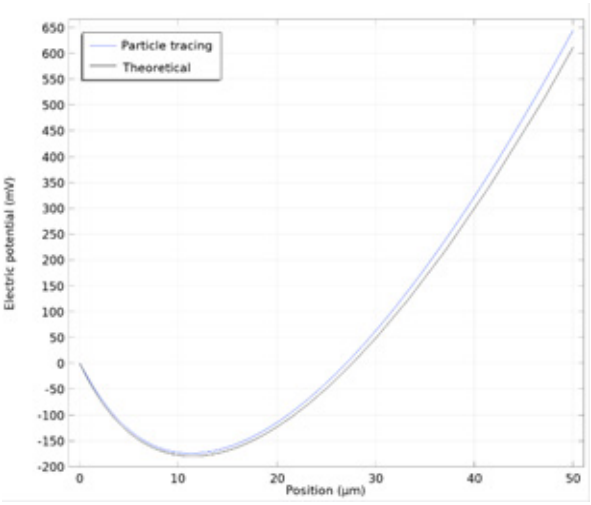


Figure 5. The electric potential across the planar diode for Tantalum at the 2400 K temperature regime.

displayed in Table 4. The potential difference generated within the diode is congruent with the work function of the material. Cerium hexaboride is found to perform better than Lanthanum Hexaboride in the 1500 K temperature regime, while Tungsten was found to perform better than Molybdenum in the 2500 K temperature regime. The saturation current appears to be fairly the same abiding by the diode characteristics.

3.2 Current Saturation Simulation

The saturation current is found by verifying the current-voltage (I-V) characteristics of the diode. Simulations were performed to obtain the magnitude of the current for a given applied voltage. The I-V characteristics of the emitter materials are tabulated in Table 4, in 15 V increments.

Table 5. The output of the current-voltage simulation for the Inserts

Potential (V)	LaB6 (A)	CeB6 (A)	Ta (A)	Mo (A)	W (A)
15	0.0192	0.0185	0.0205	0.0205	0.0215
30	0.048	0.0485	0.0514	0.05	0.0518
45	0.0841	0.0861	0.0899	0.0861	0.0887
60	0.1268	0.1273	0.1332	0.1148	0.1318
75	0.1733	0.1666	0.1815	0.1148	0.1815
90	0.2243	0.2249	0.2341	0.1148	0.2338
100	0.255	0.2627	0.2698	0.1148	0.2699
125	0.286	0.3634	0.3735	0.1148	0.3707
150	0.286	0.332	0.4845	0.1148	0.4768
175	0.286	0.8278	0.8006	0.1148	0.583
200	0.286	0.5877	0.9529	0.1148	0.583
250	0.286	0.986	1.1463	0.1148	0.583
300	0.286	0.986	1.2224	0.1148	0.583
350	0.286	0.986	1.2224	0.1148	0.583
400	0.286	0.986	1.2224	0.1148	0.583
500	0.286	0.986	1.2224	0.1148	0.583

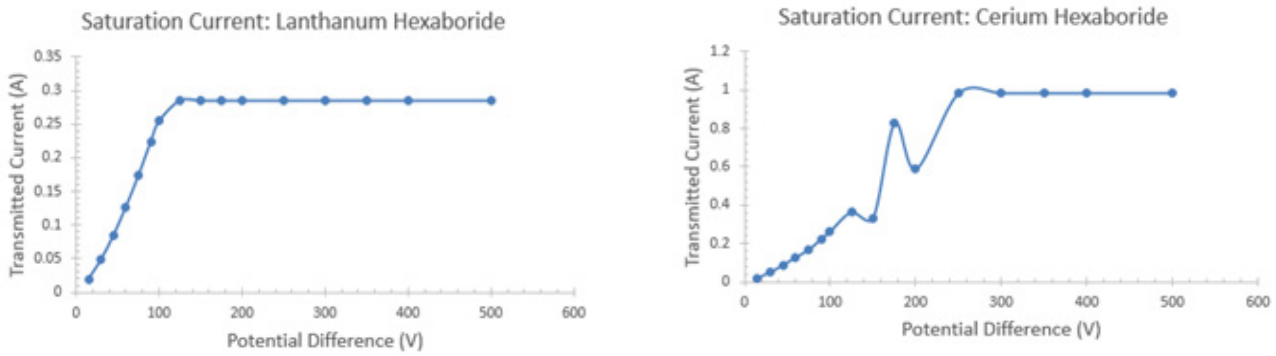


Figure 6. Lanthanum hexaboride (left) and Cerium hexaboride (right) saturation currents at the 1500 K temperature regime.

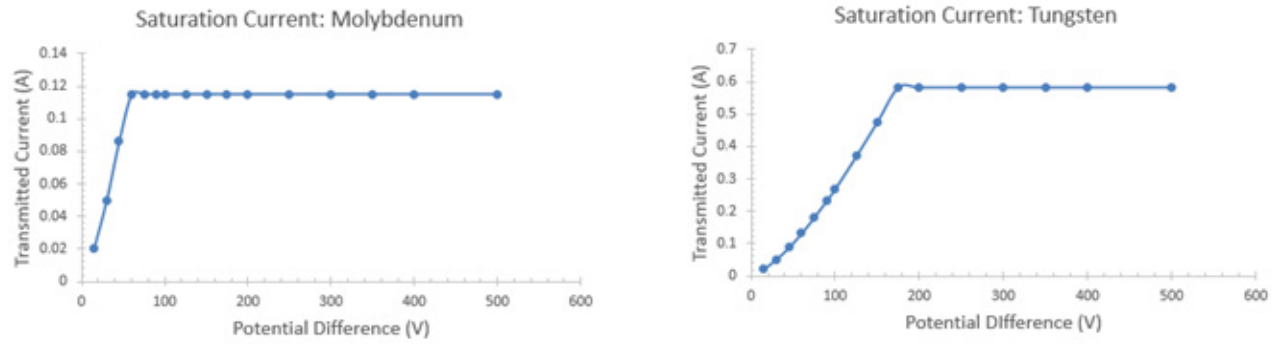


Figure 7. . Molybdenum (left) and Tungsten (right) saturation currents at the 2500 K temperature regime.

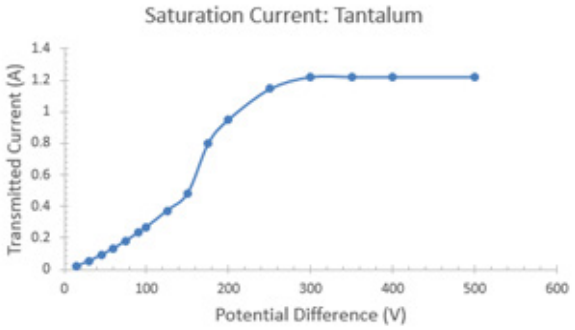


Figure 8. Tantalum saturation current at temperature 2400 K.

The saturation current is obtained by taking the transmitted current on the Y-axis and the potential difference between the electrodes along the X-axis. Materials with similar work functions have been paired into the same temperature regime to illustrate a contrast in their performance. The obtained graphs are illustrated in Figures 6 to 8 for the system of thermionic emitters under consideration.

3.2 Lanthanum Hexaboride Characteristics

Simulations have been performed to characterise Lanthanum hexaboride as a case study using the COMSOL benchmark model. The space charge between the plates due to the thermoelectricity is simulated. Figure 9(a) represents electric potential and Figure 9(b) represents electric field within the planar diode. To visualise the electrical properties in the computational domain, two perpendicular slices intersecting the centre are created in the x and z directions.

Figures 9 and 10 depict the electric field and the trajectories of the emanating electrons due to the thermionic emission of Lanthanum hexaboride modelled at 1500K. The charged particle tracing module in COMSOL

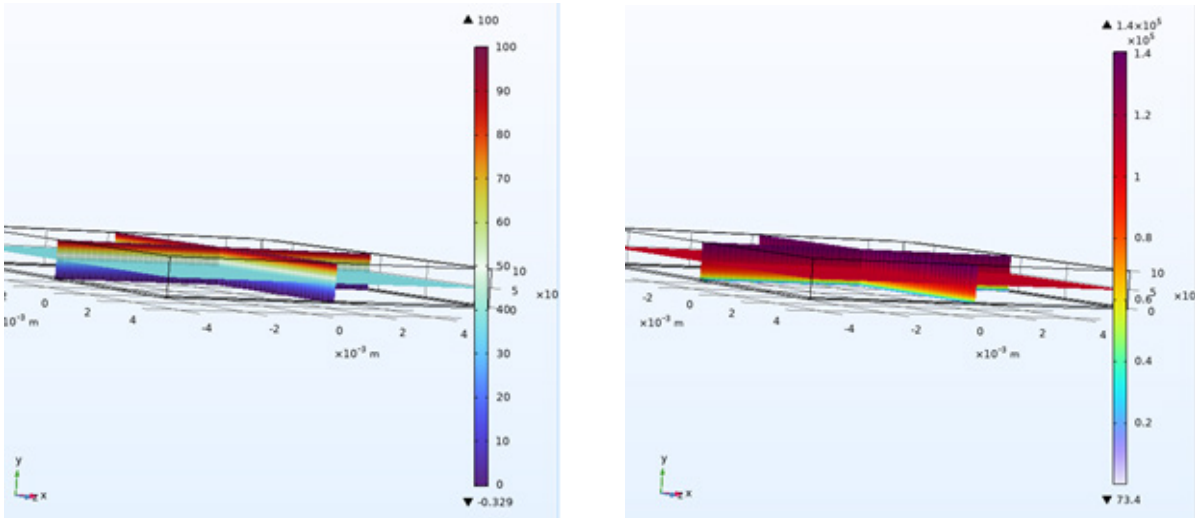


Figure 9. Visualisation of electrical parameters of Lanthanum hexaboride by taking two perpendicular slices in the computational domain **(a)** Electric potential [V] **(b)** Electric field [V/m]

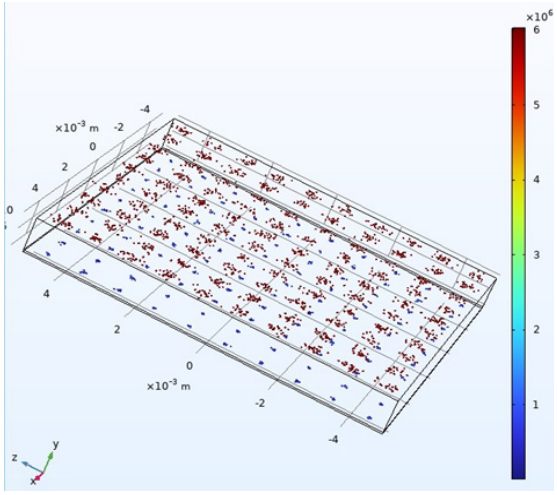


Figure 10. Particle velocity [m/s] contour of Lanthanum hexaboride hot cathode.

is used to map particle velocities and the trajectories of moving particles. The charged particle tracing module is used to characterize the emissions interaction with the developed space charge intensity. The output in Figure 10 shows the total particles at equidistant particle positions across the dimensions of the planar diode. The simulation is set to generate the number of particles at 100 particle position, spaced equidistant at 0.1 microsecond. It is the flow of these emanating electrons that constitute the thermoelectric current.

4.0 Conclusions

The simulation results are plotted to set up a comparative study between the different hollow cathode materials used in electric propulsion. Materials from the onset of electric propulsion, like Tungsten, have been included in the study to illustrate the evolution in material efficiency. As the simulations suggest, Lanthanum hexaboride and Cerium hexaboride prove to be ideal thermionic emitters due to their low work function. Furthermore, the low work function has been able to generate an observable potential drop in the 1500 K temperature regime. Tantalum in the 2000K temperature regime is found to perform moderately better in comparison to Molybdenum and Tungsten, which are simulated under the 2500K temperature regime.

Cerium hexaboride proves to perform relatively better than other emitters in the simulations. In addition to its lower work function, its larger magnitude of transmitted current for a given potential difference identifies it as a more efficient thermionic emitter. Furthermore, Cerium hexaboride is capable of operating under lower temperature regimes in comparison to Tantalum, Tungsten and Molybdenum. In addition, the material properties of Cerium hexaboride such as density and melting point are higher than that of Lanthanum hexaboride. Thus, Cerium hexaboride proves to be an

emerging alternative as an effective thermionic emitter for extreme space environments.

5.0 Acknowledgements

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