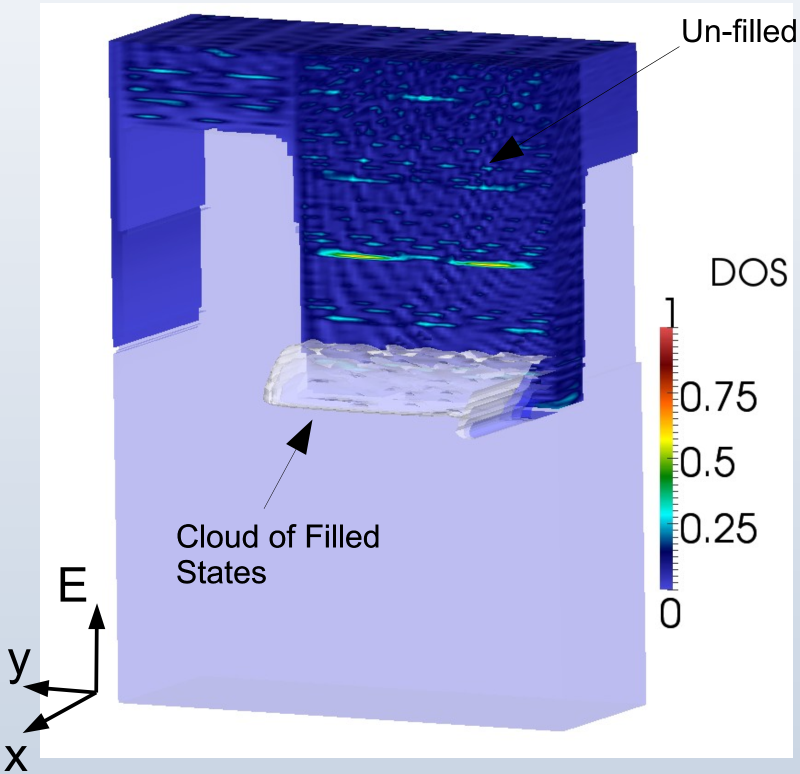
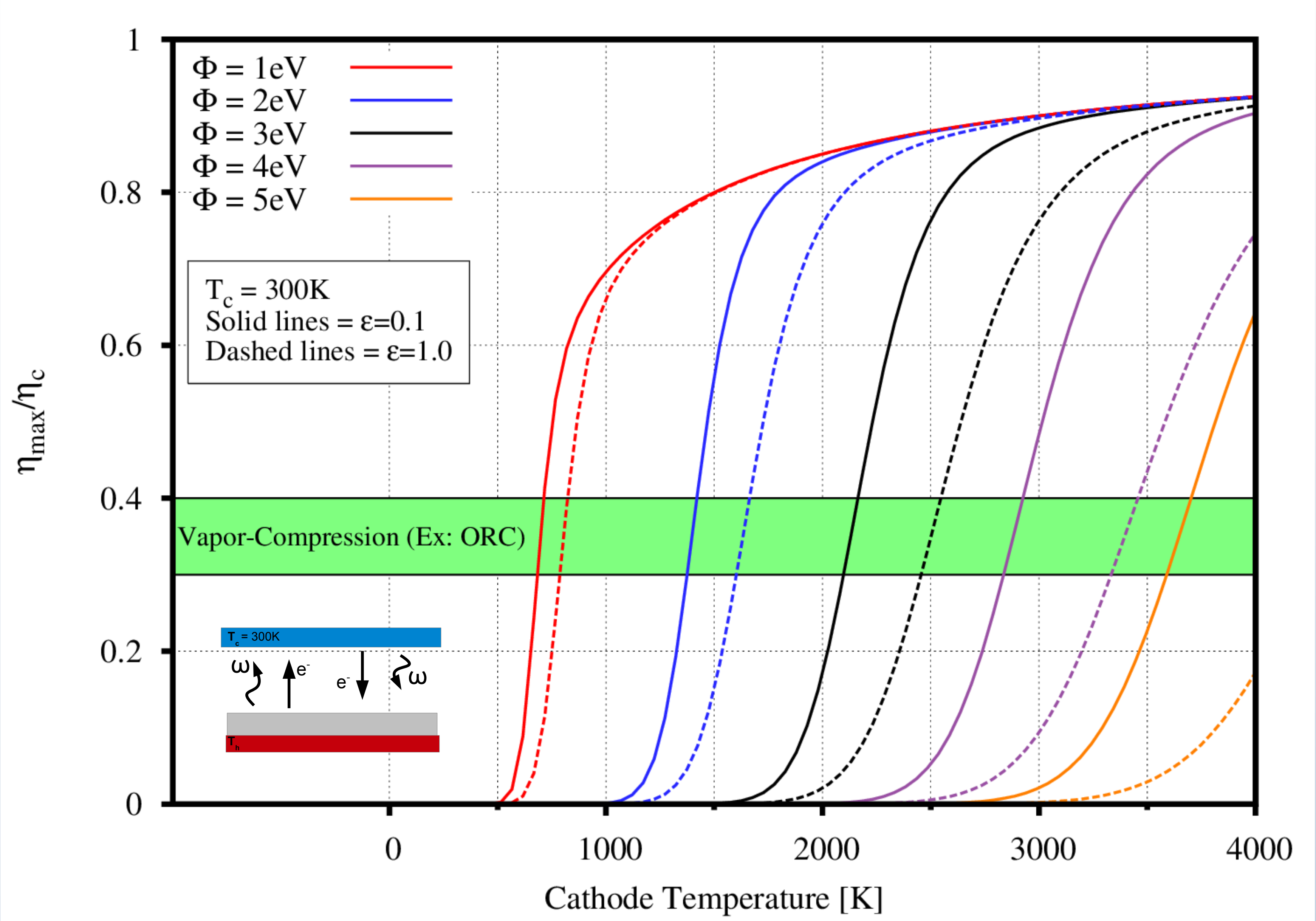
Understanding the Role of Confined Carriers in Nanotipped Thermionic Emitters



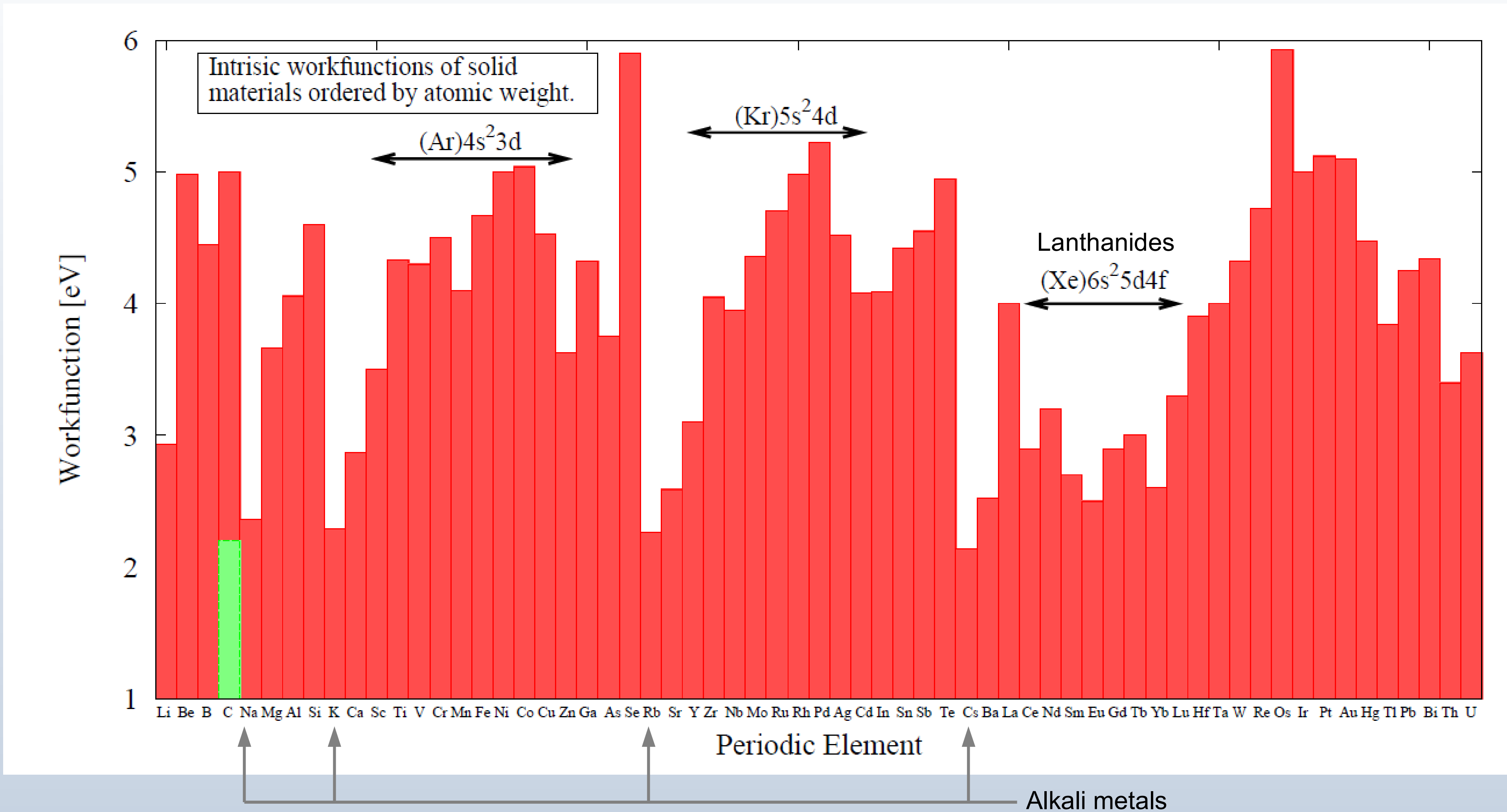
NASA Thermionic Workshop – Oct 2014
Dr. Terence Musho
West Virginia University

Conversion Efficiency of Thermionic Emitters



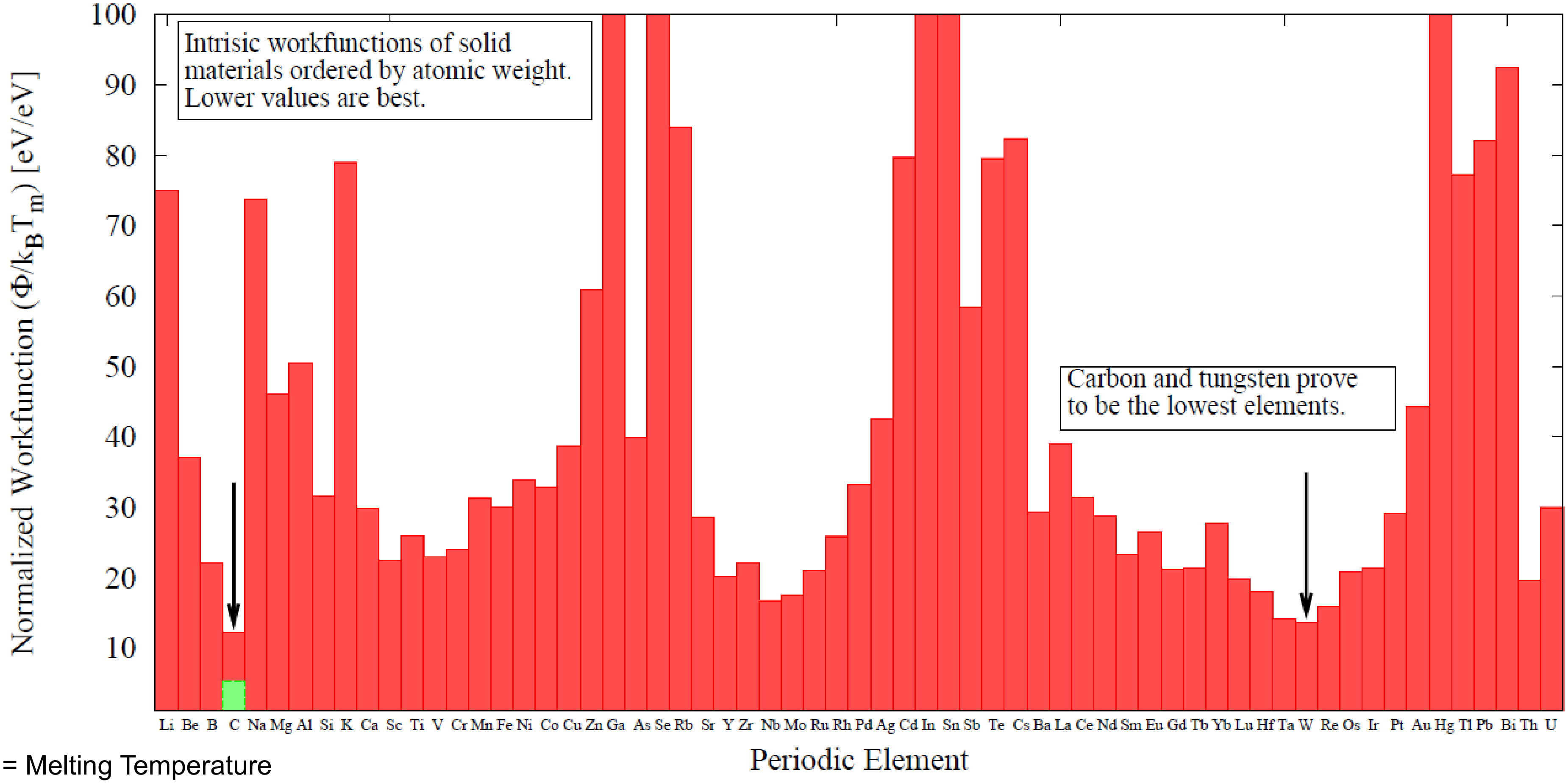
Low work function or high operating temperature to obtain comparable efficiencies to Organic Rankine Cycles (ORC).

Periodic Table Perspective of Work functions



Transition metals have increasing trend as orbitals fill. Alkali metals have lowest work function values. Lanthanides has moderate workfunction.

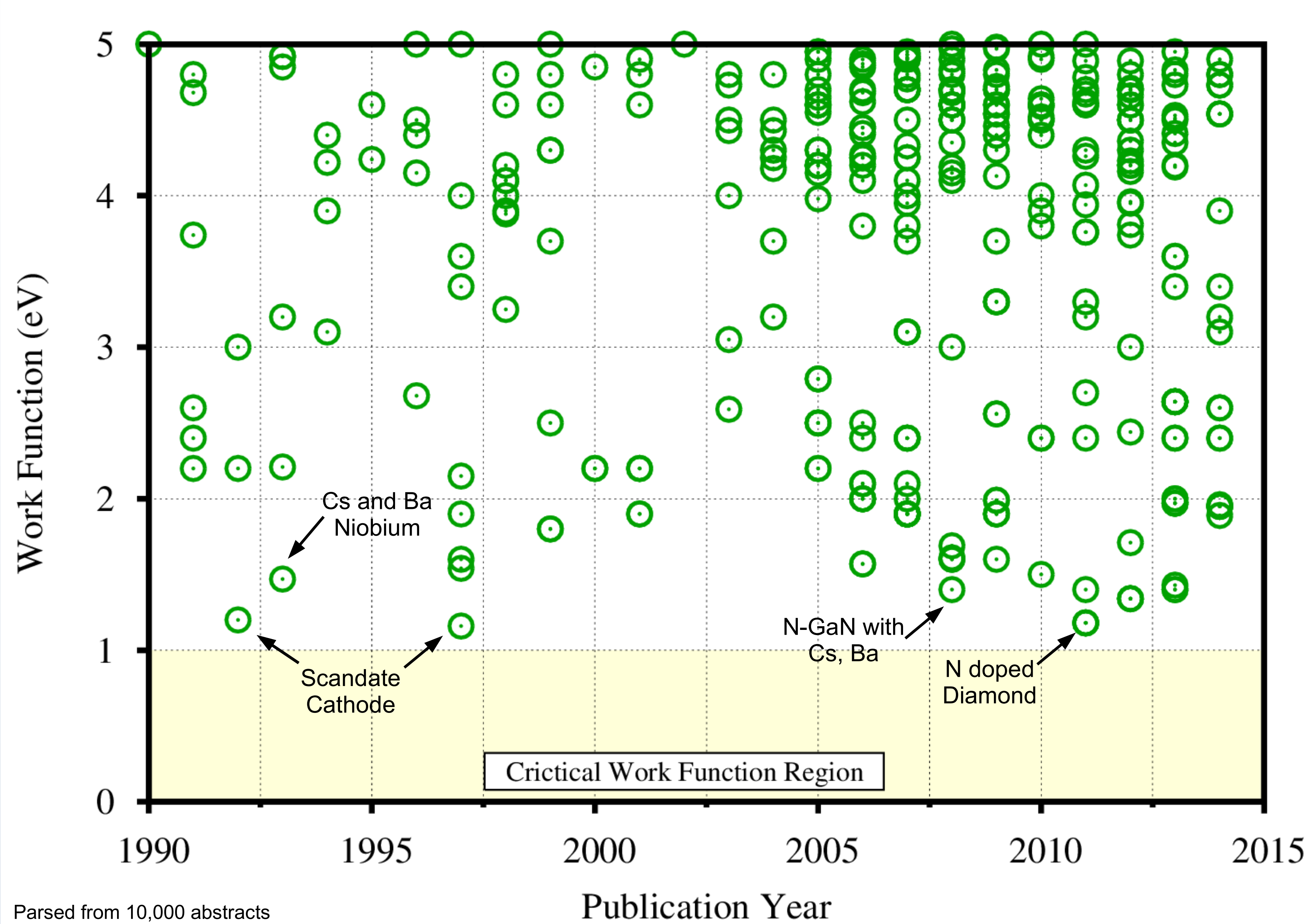
Periodic Table Perspective of Work functions



T_m = Melting Temperature

Dividing the work function by the melting temperature reveals carbon and tungsten to be the lowest.

Historical Literature Perspective of Work functions



Over the last 25 years there has not been a huge improvement in identifying lower work function materials. Scandate and diamond prove to be lowest.

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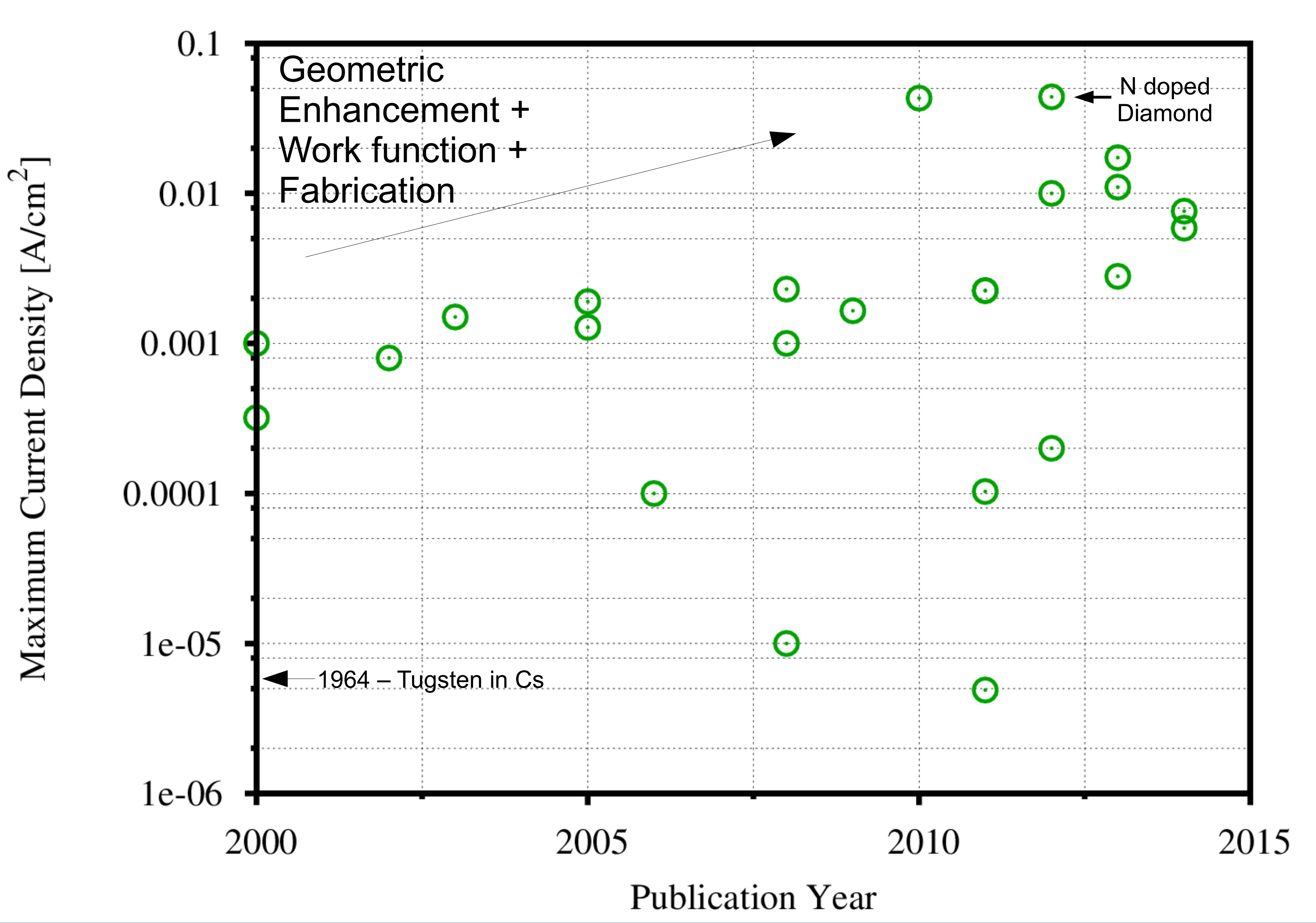
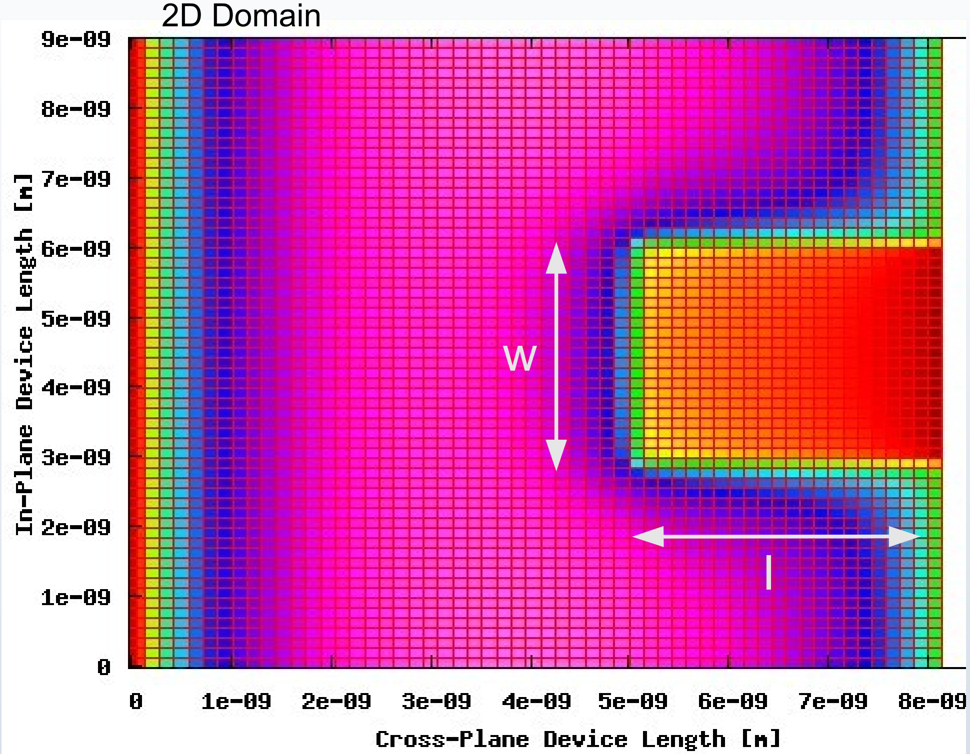
Historical Literature Perspective of Current Density



Over the last decade there has been a significant increase in current density. This is reasoned to be a results of geometric and fabrication influences.

Understanding the Role of Confined Carriers

2D Domain



Self-Consistent Poisson Loop

$$H = \frac{-\hbar}{2m} \nabla^2 + V^{eff}[n]$$

$$\nabla^2 V^{eff}[n] = \frac{\varrho}{\varepsilon}$$

HF

2D Effective Mass Hamiltonian
Basis of Lowest Conduction Band

$$H = \frac{-\hbar}{2m} \nabla^2 + V^{eff}[n]$$

$$G = EI - H + V + \Sigma_1 + \Sigma_2$$

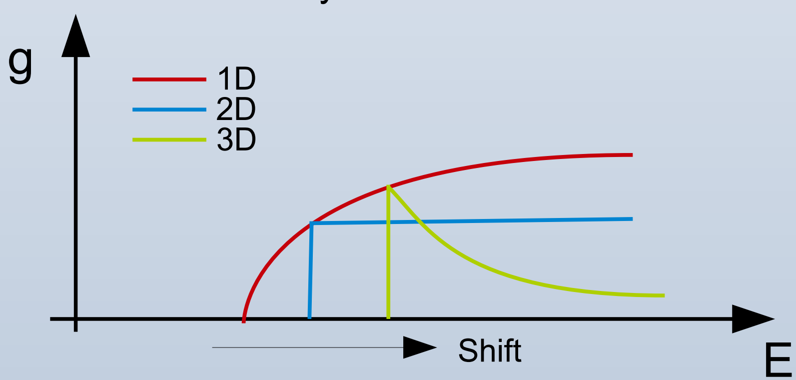
$$\Xi = Tr[\Gamma_1 G G^t \Gamma_2]$$

Fermi-Dirac Dist.

$$I = \int_0^\infty \frac{2e^2}{h} \Xi (f_2 - f_1) dE$$

Transmission

Confined Density of States



It is hypothesized that that the spatially confined carriers in nanotip can lead to localized field enhancement.

Potential

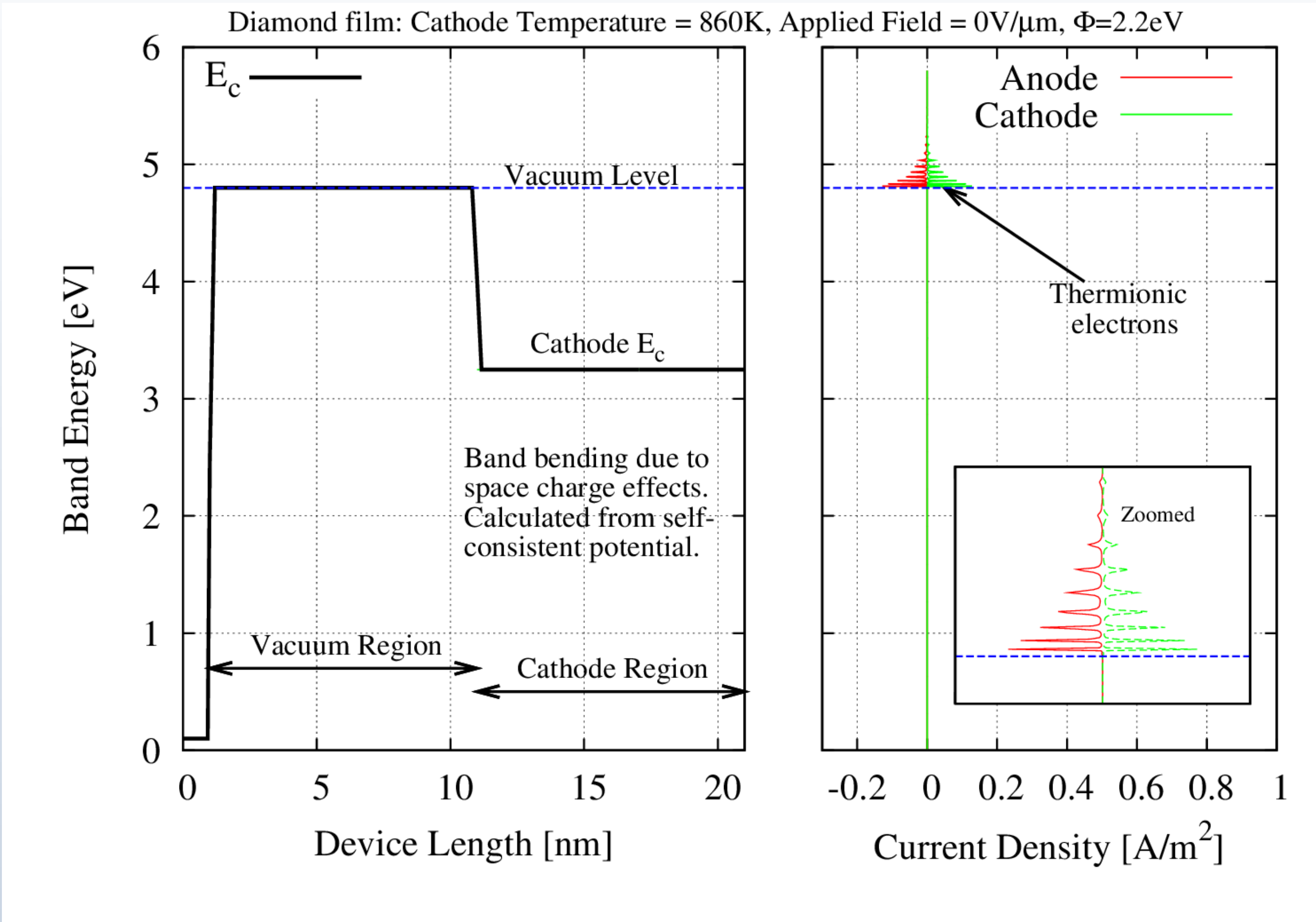
$$\nabla^2 V^{eff}(x, y) = \frac{\varrho(x, y)}{\varepsilon}$$

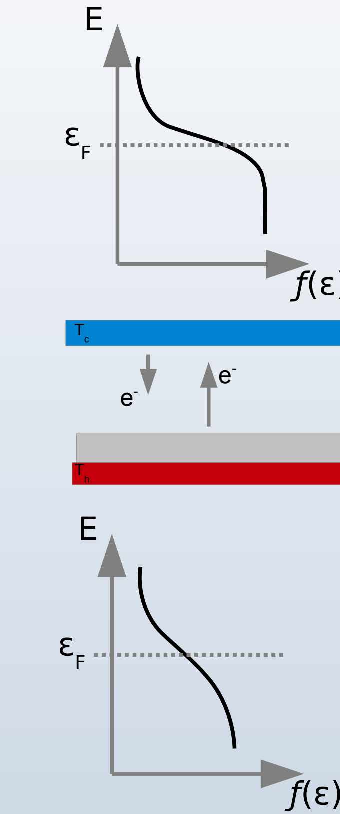
Charge Density

Dielectric Constant

A two dimensional quantum model is used to predict the influence of the tip geometry on the emission characteristics.

Thermionic Emission

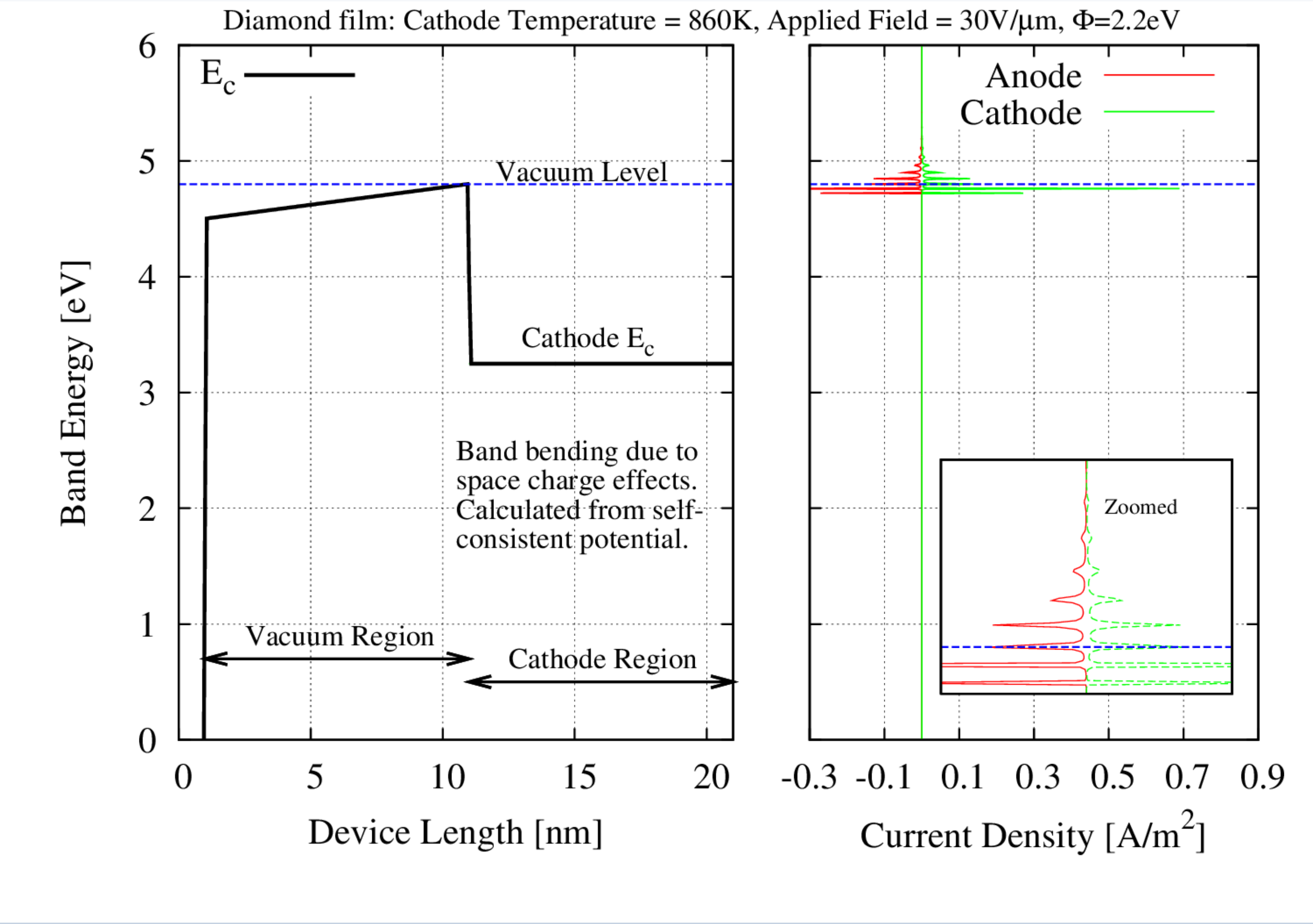


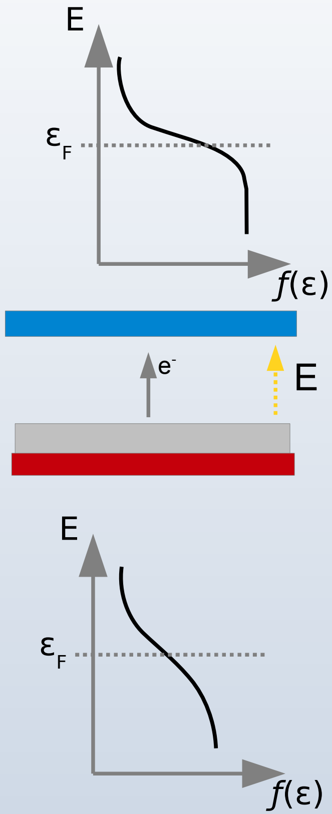


$$I = \int_0^\infty \frac{2e^2}{h} \Xi (f_2 - f_1)\, dE$$

In pure thermionic emission the current is above the vacuume level. Discrete states result in discrete peaks in current.

Thermal-Field Emission Model





In thermal-field emission tunneling current below the vacuum level results in increased overall current.

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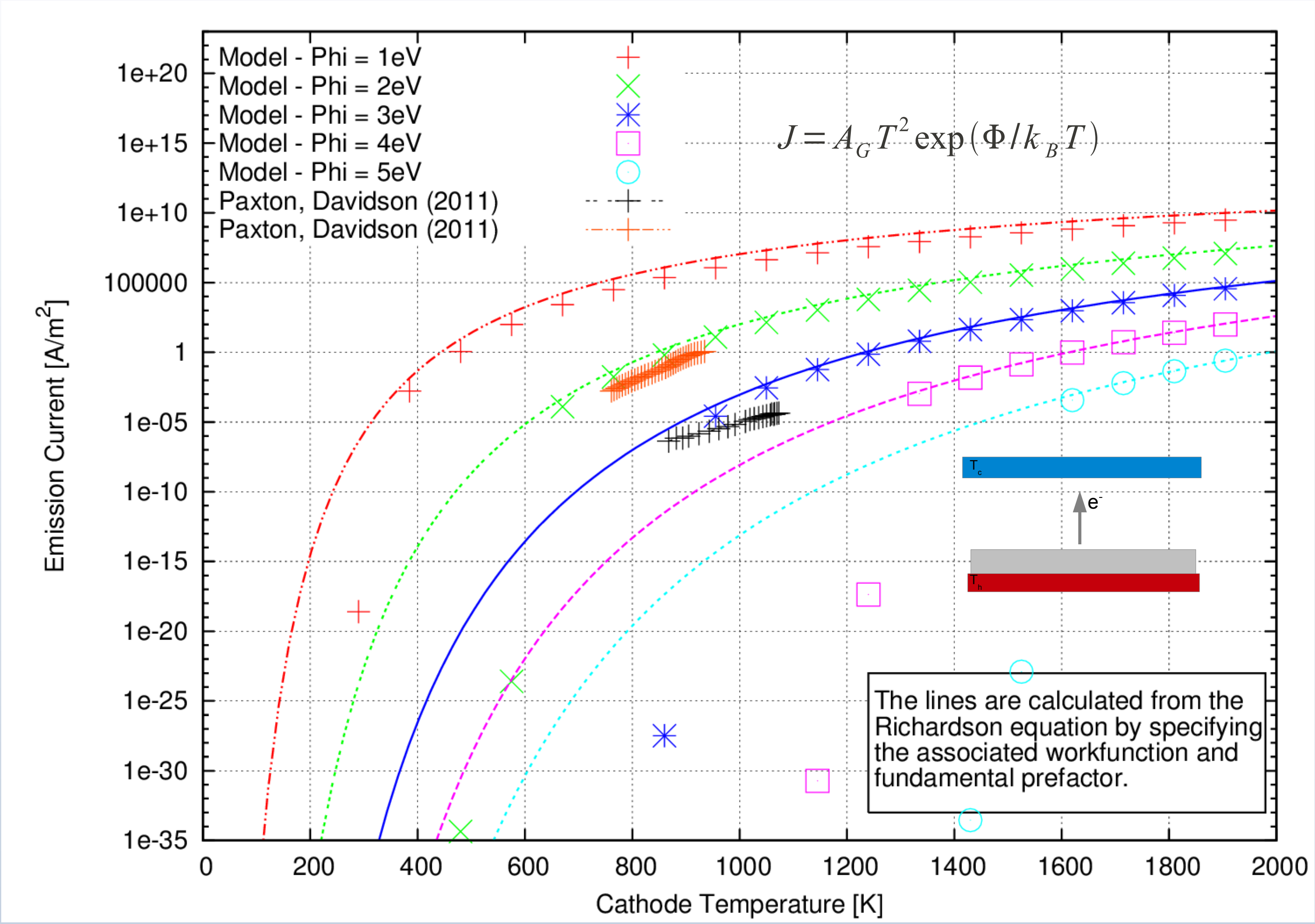
Thermionic Emission Thin Film



Thermionic model provides more accurate description of emission current along with the ability to predict the on-set of thermionic emission.

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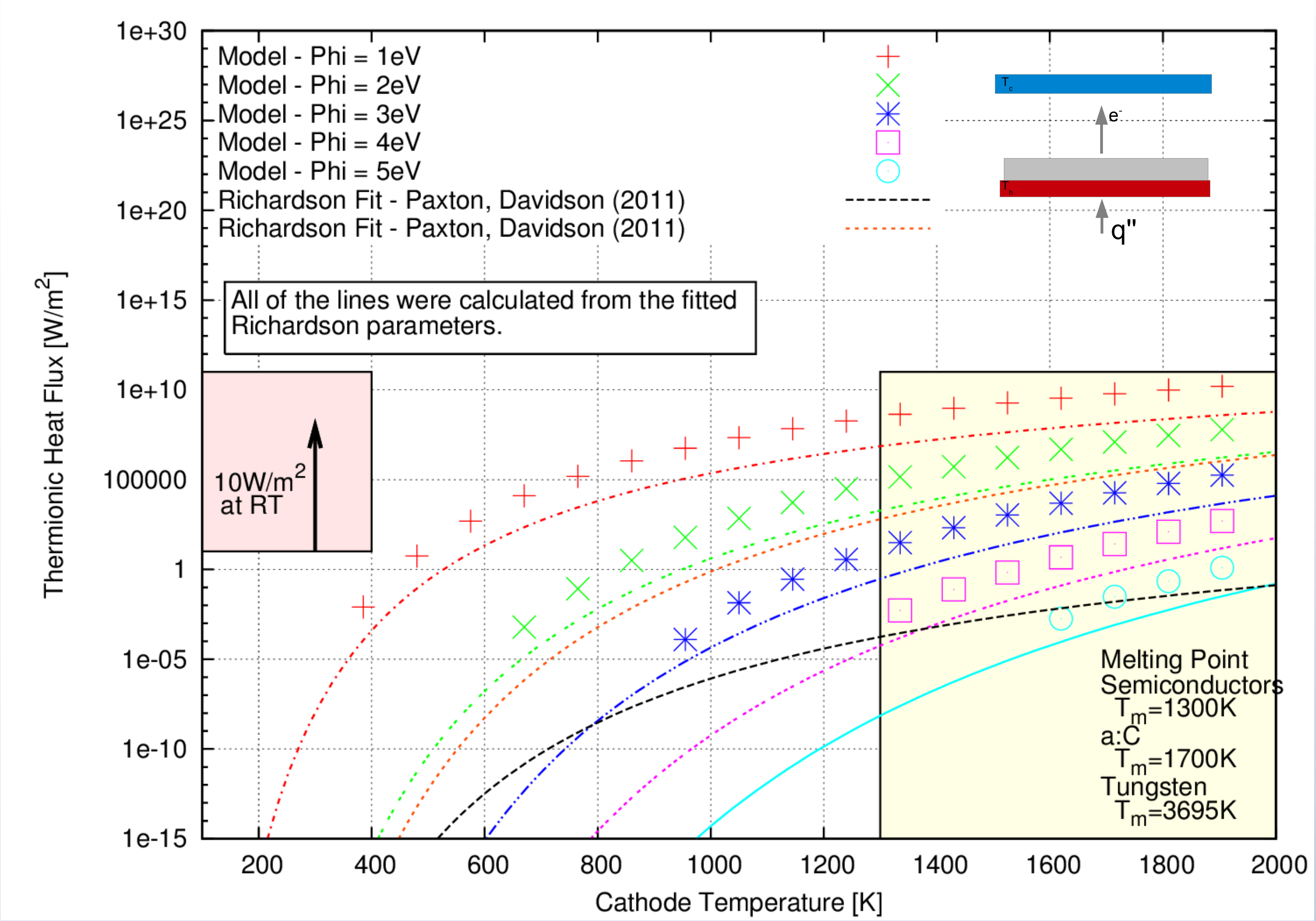
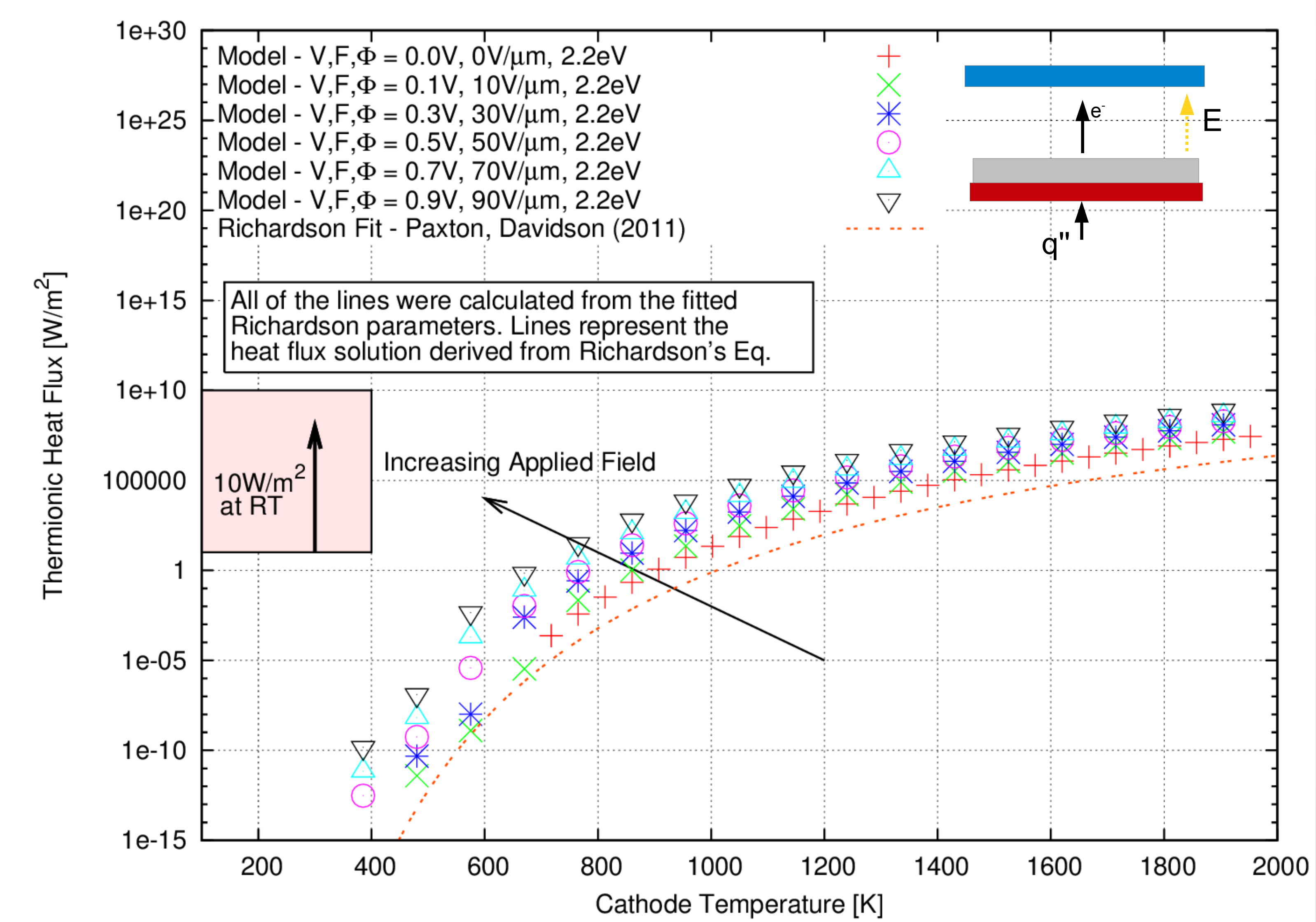
Thermionic Heat Flux or Power from Thin Film



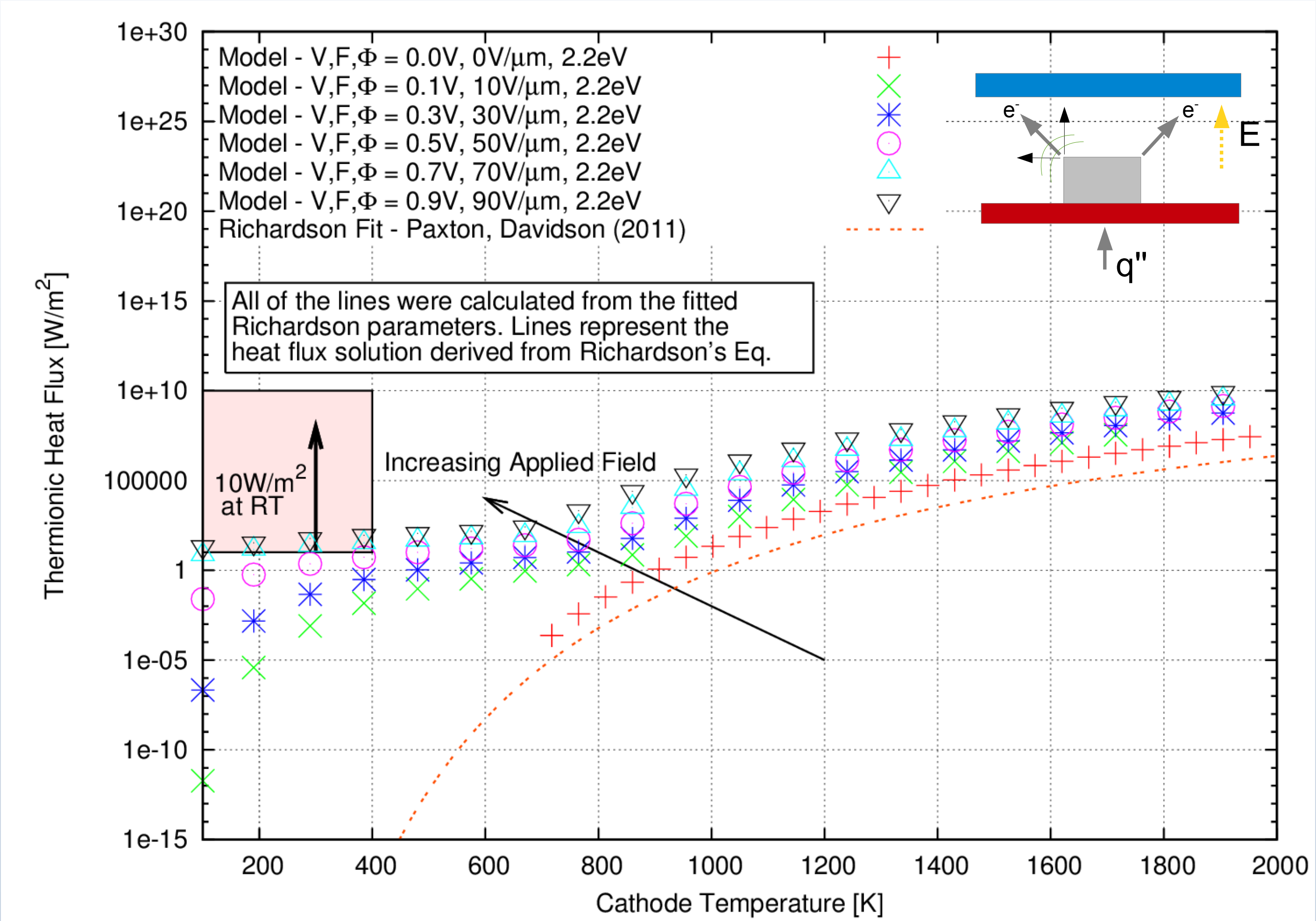
The electronic heat flux or thermionic power can be predicted using the calculated spectral density and kinetic energy of carriers.

Thermal-Field Heat Flux or Power from Thin Film



Under combined thermionic and field emission the current increases with increase tunneling current due to band bending.

Thermal-Field Heat Flux or Power from Thin Film



The emission power results in lower temperature field emission as a results of the field enhancment of the nanotip geometry.

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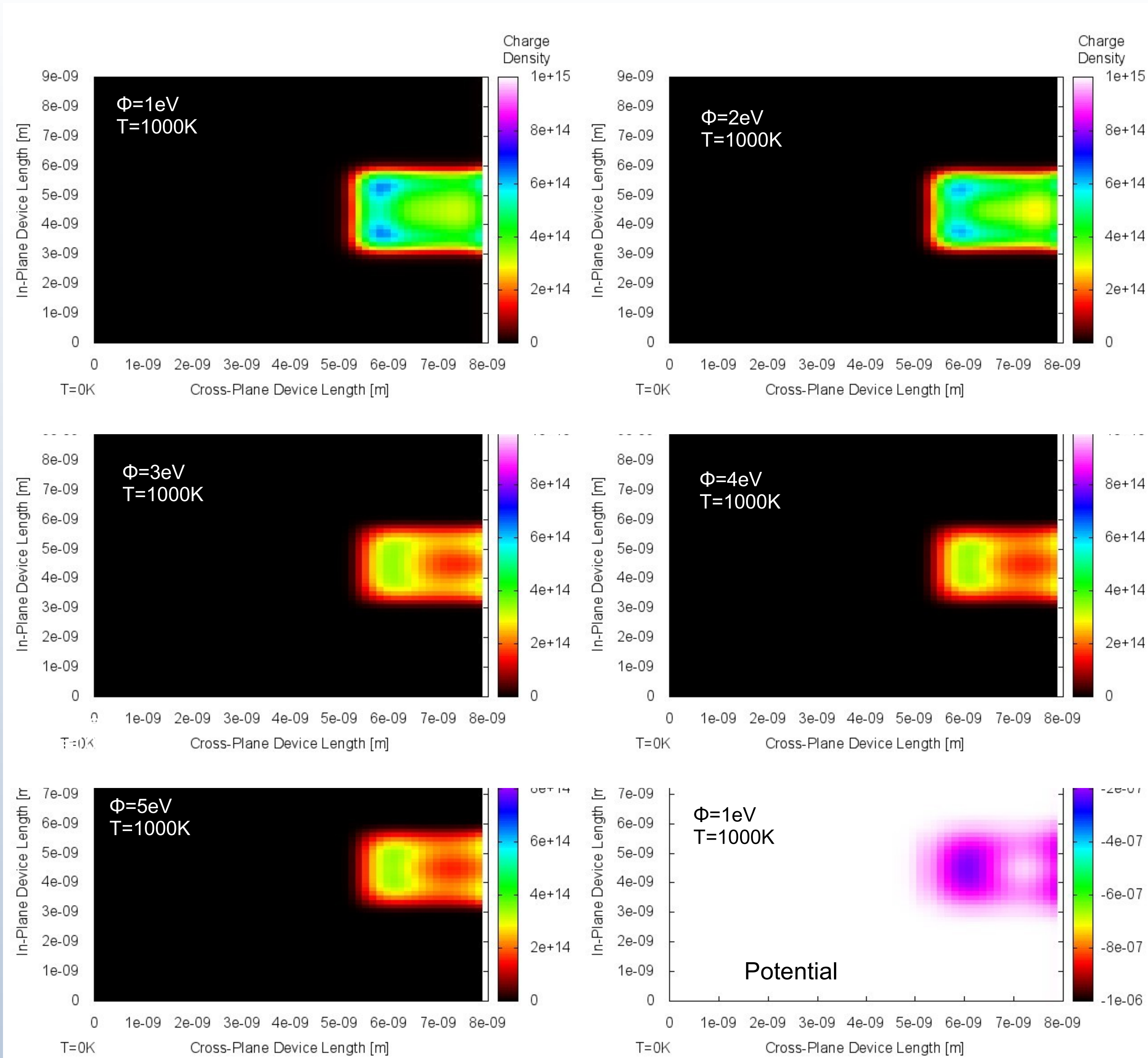
Nanotipped Spatial Charge Density – Tip Width



Nanotip Geometry
w=2nm
l=2nm

Localization of charge near corners and end. Changer in intensity a result of Fermi distribution. Change in potential localized near tip. Low carrier population due to size.

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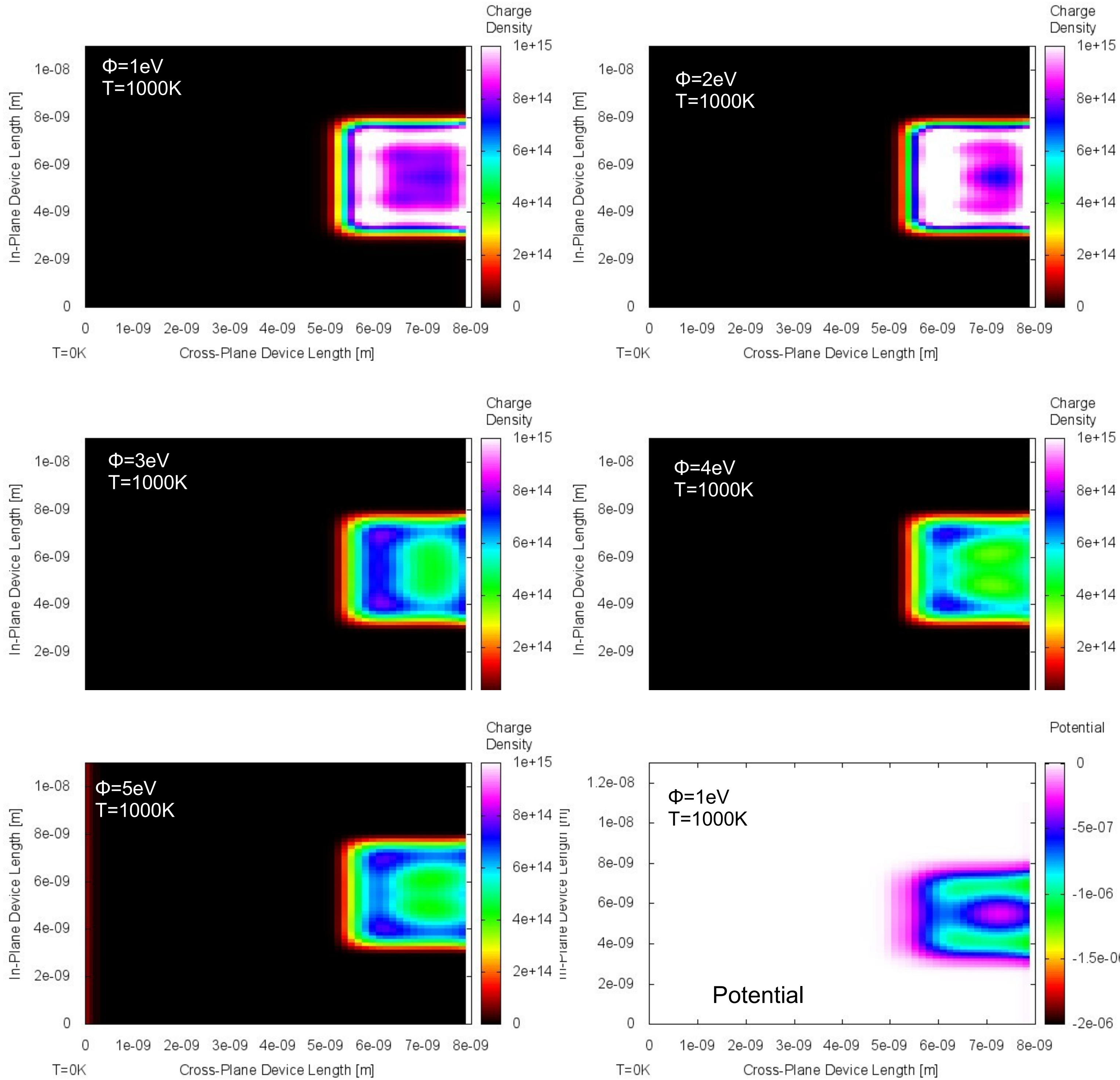
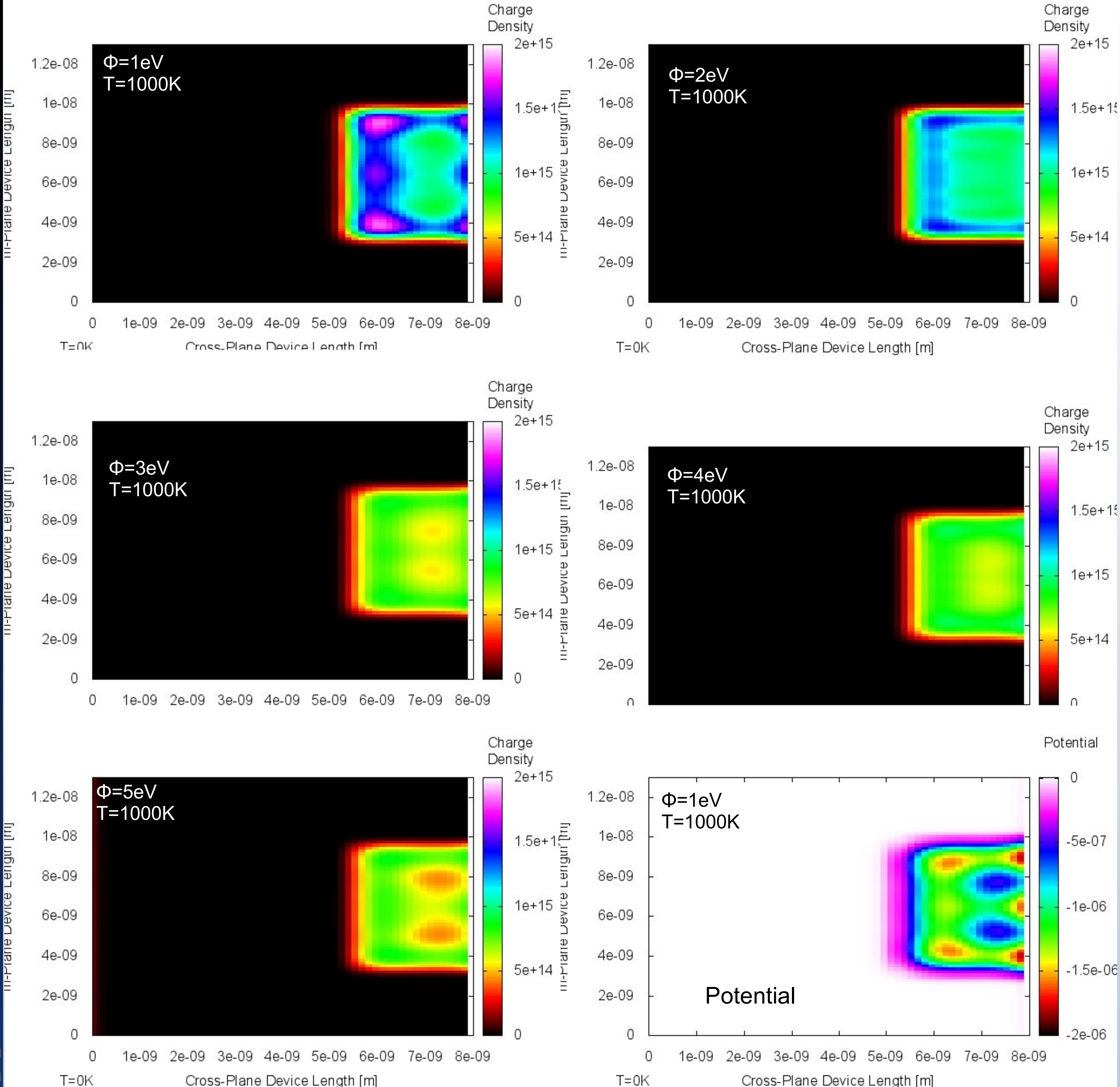


Nanotip Geometry
w=4nm
l=2nm

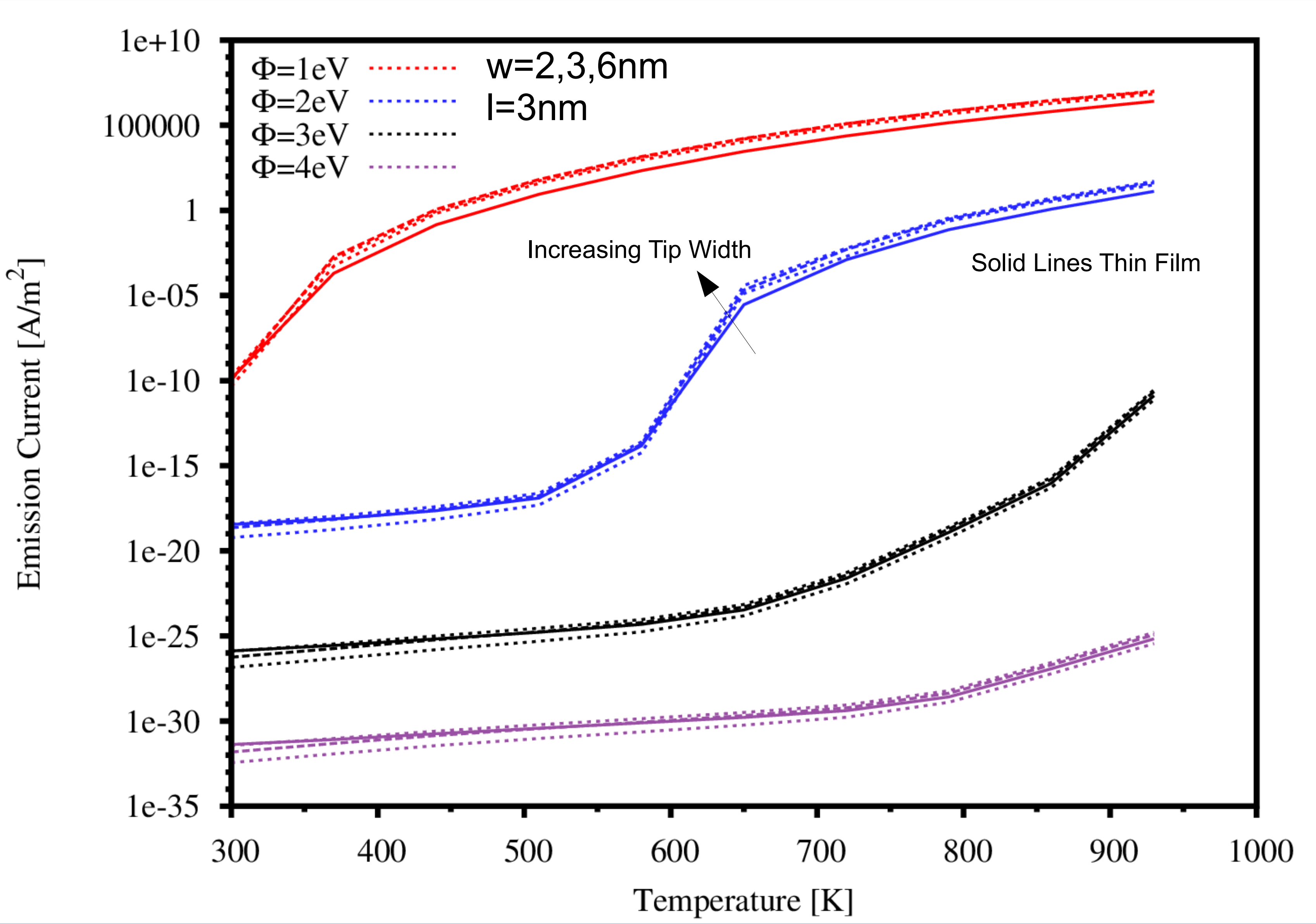
Localization of charge near edges an corners. Change in potential localized near sides of nanotip. Carrier concentration increase as confinement relaxes in transverse.



Nanotip Geometry
w=6nm
l=2nm

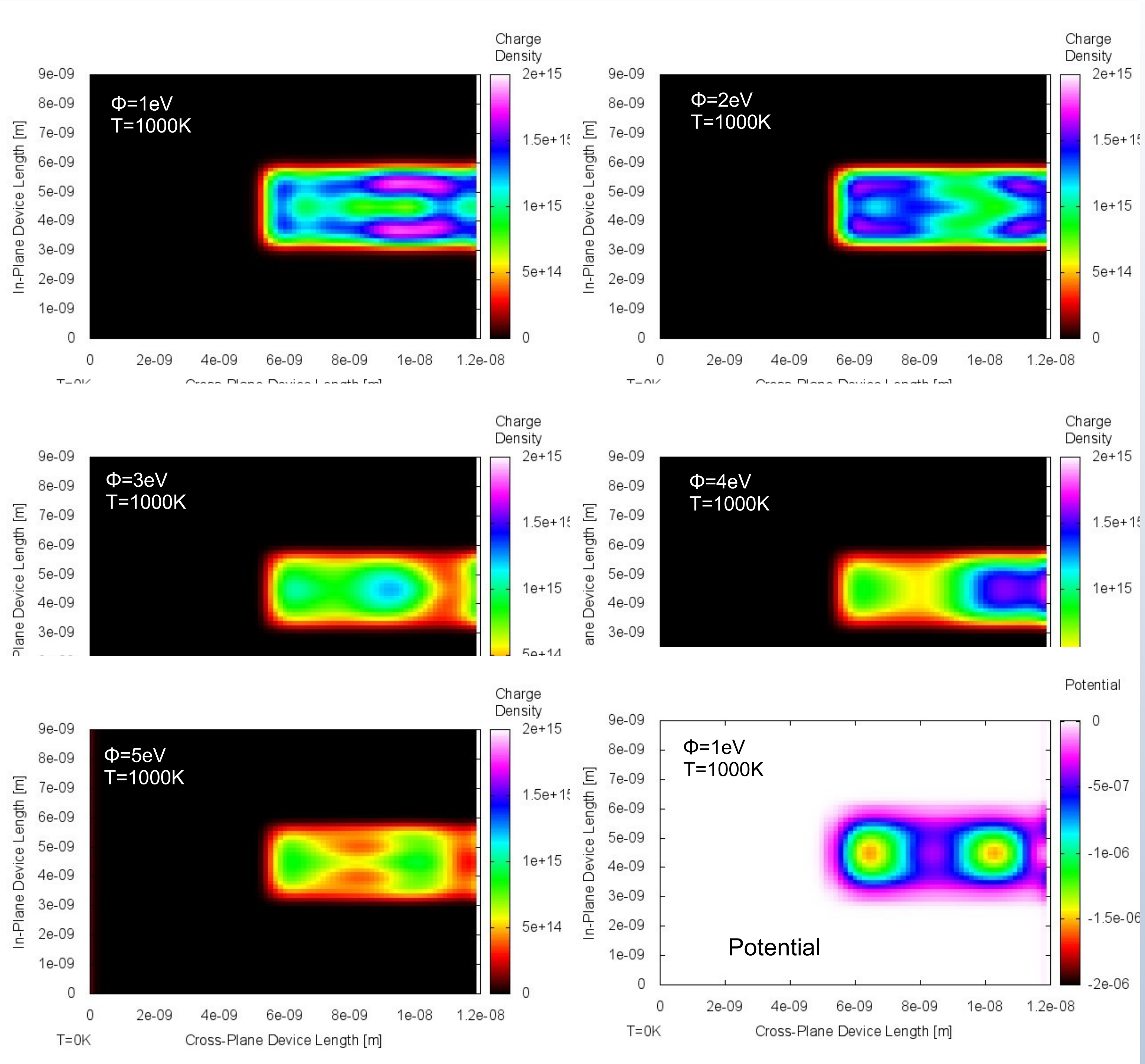
As transverse confinement relaxes the charge density increases and becomes more continuous. Potential plot shows peaks near edge and base.

Nanotipped Spatial Charge Density – Tip Width



Slight increase with tip width. Reasoned to be heavily influences by charge density.

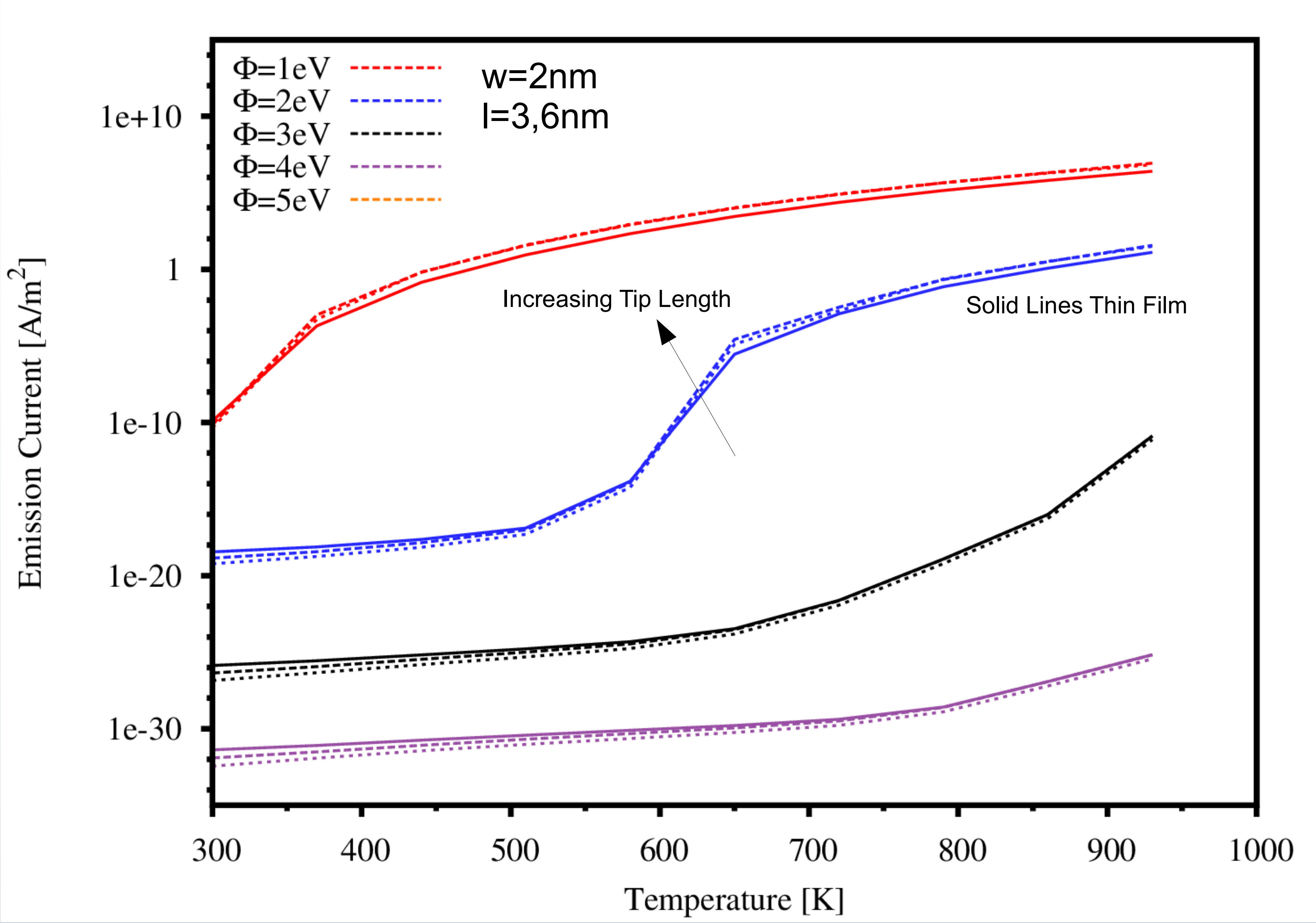
Nanotipped Spatial Charge Density – Tip Length



Nanotip Geometry
w=2nm
l=6nm

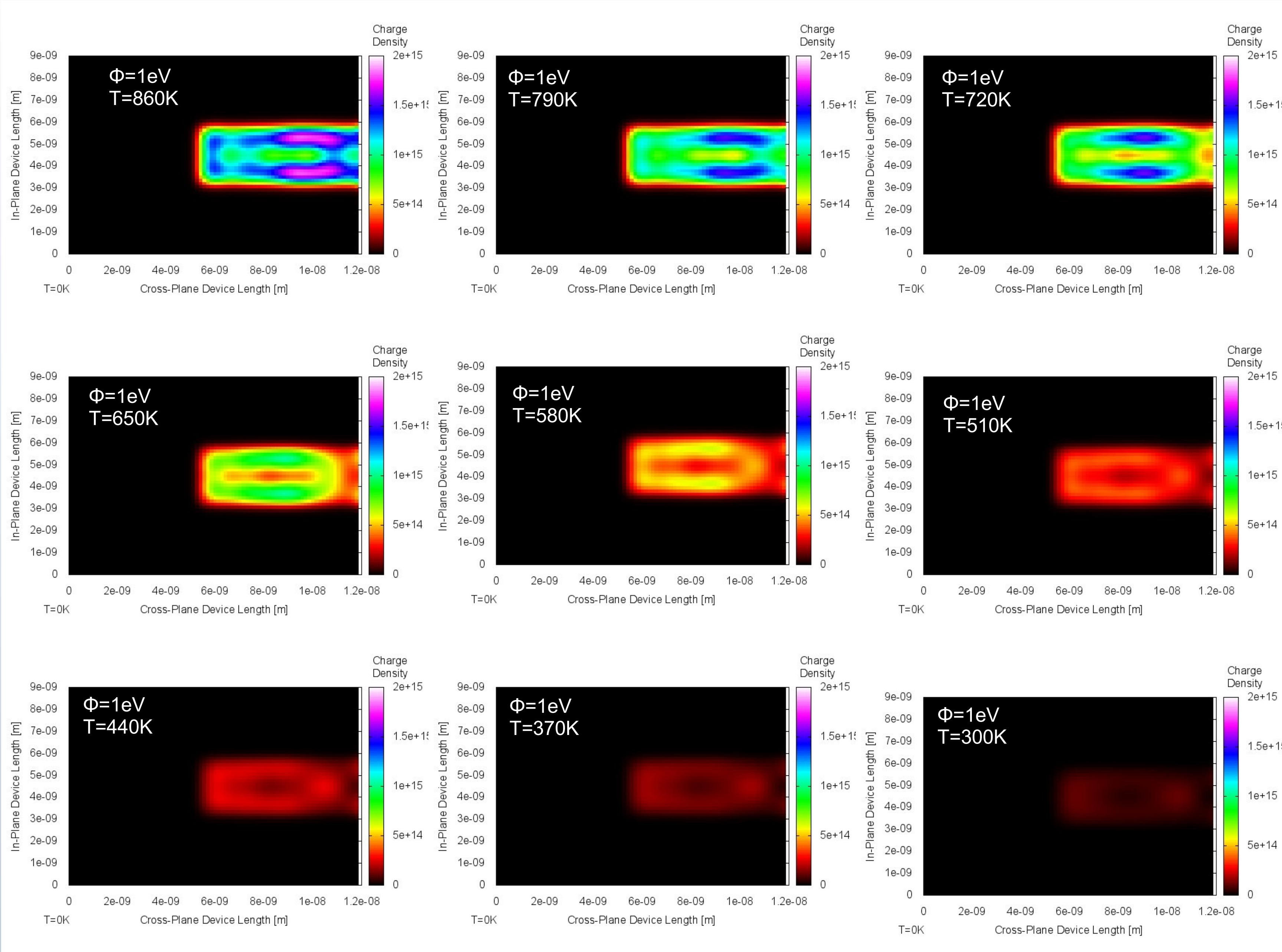
As longitudinal confinement relaxes the charge have two regions of higher density charge. Potential plot shows a clear view bi-modal distribution.

Nanotipped Spatial Charge Density – Tip Length



Increase emission with tip emitter compared to thin film however the emission is not heavily dependent on the length.

Nanotipped Spatial Charge Density – Temperature



Nanotip Geometry
w=2nm
l=6nm

Highest charge distribution near edge and scales by Fermi Dist.

Conclusion

Workfunction values have been steady over the past 25 year however there has been a large improvement of current density. This was reasoned to be a result of fabrication (lower interface resistance) and geometric improvements.

The thermionic emission current did have a marginal improvement with the addition of the tip (2-6nm).

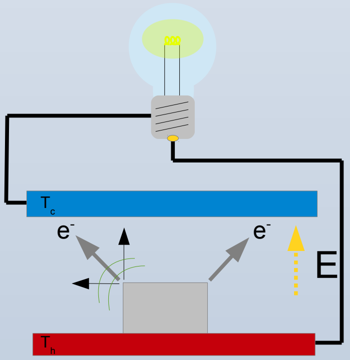
The governing factor for the improvement was more than likely the increase in charge density as the confinement relaxed states. The relaxation in the transverse direction proved most beneficial.

Density plots confirm that the charge density within the nanotip are not localized exclusively near the tip. This might be an avenue for further investigation.

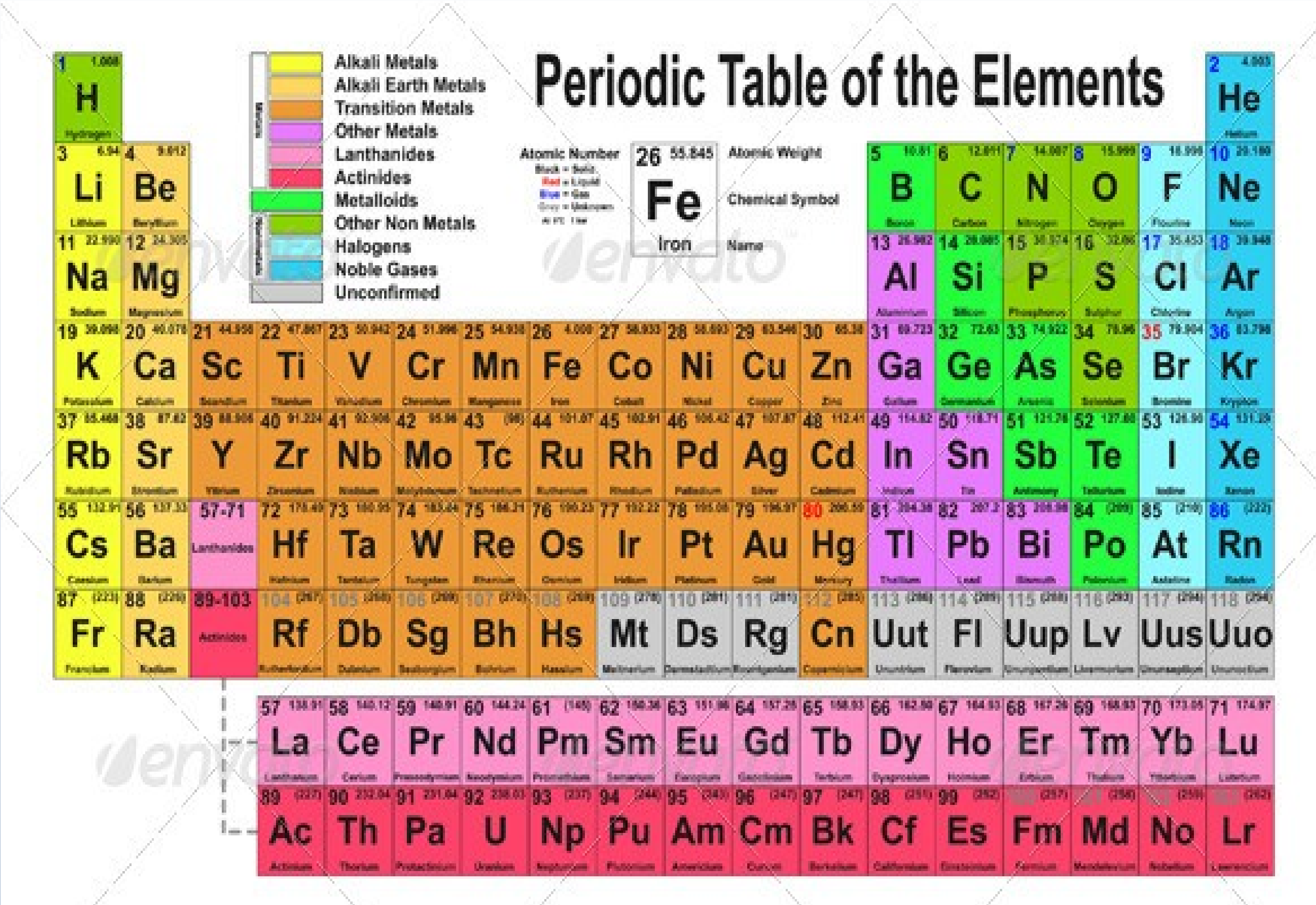
Future investigations will look at larger tip geometries approaching the continuum regime. Run GPU code on XCEDE.

Investigate specific device constructions. Ex: material, dimensions, gate voltage.

Look at the the confinement of a wide band gap material on surface.



The End


Periodic Table of the Elements
Alkali Metals
Alkali Earth Metals
Transition Metals
Other Metals
Lanthanides
Actinides
Metalloids
Other Non Metals
Halogens
Noble Gases
Unconfirmed
Atomic Number
26 55.845
Fe
Iron
Atomic Weight
Chemical Symbol
Name
1 H Hydrogen
2 He Helium
3 Li 4 Be 5 B 6 C 7 N 8 O 9 F 10 Ne
11 Na 12 Mg 13 Al 14 Si 15 P 16 S 17 Cl 18 Ar
19 K 20 Ca 21 Sc 22 Ti 23 V 24 Cr 25 Mn 26 Fe 27 Co 28 Ni 29 Cu 30 Zn 31 Ga 32 Ge 33 As 34 Se 35 Br 36 Kr
37 Rb 38 Sr 39 Y 40 Zr 41 Nb 42 Mo 43 Tc 44 Ru 45 Rh 46 Pd 47 Ag 48 Cd 49 In 50 Sn 51 Sb 52 Te 53 I 54 Xe
55 Cs 56 Ba 57-71 Lanthanides 72 Hf 73 Ta 74 W 75 Re 76 Os 77 Ir 78 Pt 79 Au 80 Hg 81 Tl 82 Pb 83 Bi 84 Po 85 At 86 Rn
87 Fr 88 Ra 89-103 Actinides 104 Rf 105 Db 106 Sg 107 Bh 108 Hs 109 Mt 110 Ds 111 Rg 112 Cn 113 Uut 114 Fl 115 Uup 116 Lv 117 Uus 118 Uuo
57 La 58 Ce 59 Pr 60 Nd 61 Pm 62 Sm 63 Eu 64 Gd 65 Tb 66 Dy 67 Ho 68 Er 69 Tm 70 Yb 71 Lu
89 Ac 90 Th 91 Pa 92 U 93 Np 94 Pu 95 Am 96 Cm 97 Bk 98 Cf 99 Es Fm Md No Lr