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Beta-enhanced Thermionic Diamond Energy Converters (BTDC) and Nuclear Batteries Project

NASA 2014 Workshop
Houston
14th October 2014

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Project Principal Investigator
University of Bristol
UK

Image : http://www.nasa.gov/mission_pages/sunearth/news/News090811-X1.8flare.html

OUTLINE

- PROJECT SCOPE & OBJECTIVES
- SUPPORTING WORK
- PROJECT RESULTS

Research Programme

Phase 1 — 15 months

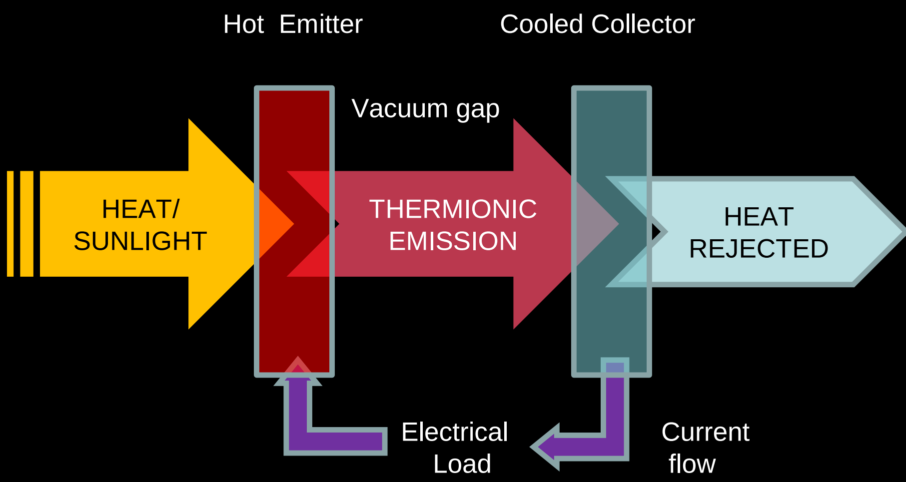
Phase 2 — 27 months

2016/Q3

WP 1	Nano/Micro-Absorbers – Surface & Bulk Doping	EE CHEM
WP 2	Diamond Electrode - Synthesis & Characterisation	CHEM/PHYS
WP 3	Fabrication of Radiation Absorbing Structures	EE CHEM
WP 4	Prototype Devices & Testing	PHYS/CHEM

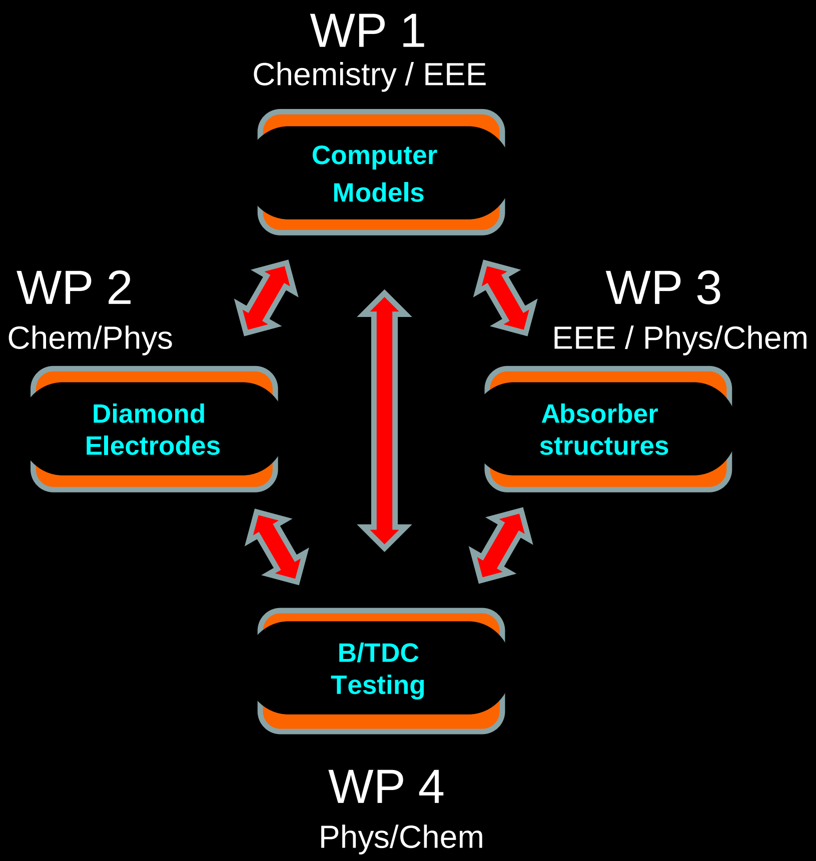
Thermionic Diamond Converter (TDC)

- Solid State Conversion of Heat / Radiation to Electrical Power
- Function of Components Parts
  - Emitter /Cathode
    - Photon absorber (input side)
    - Thermionic emitter (output side)
  - Collector /Anode
    - Electron absorber (input side)
    - Heat sink (output side)



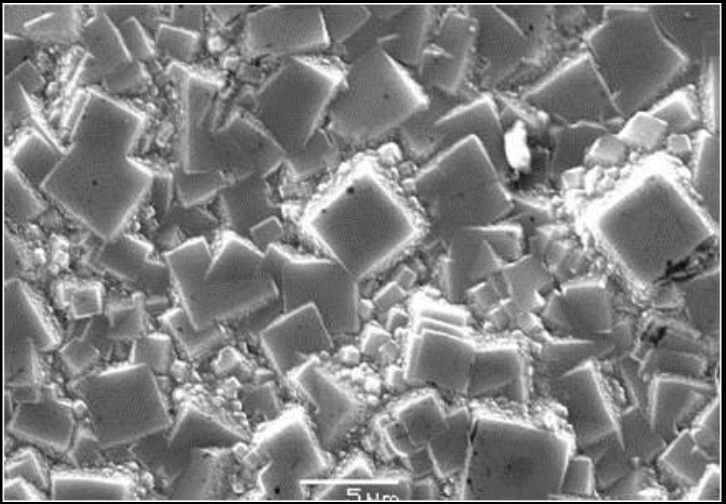
Project objectives

- High current thermionic emission from diamond
- High efficiency radiation absorbers
- Diamond solar energy converter
- Beta-enhanced thermionics
- Beta-diamond nuclear battery

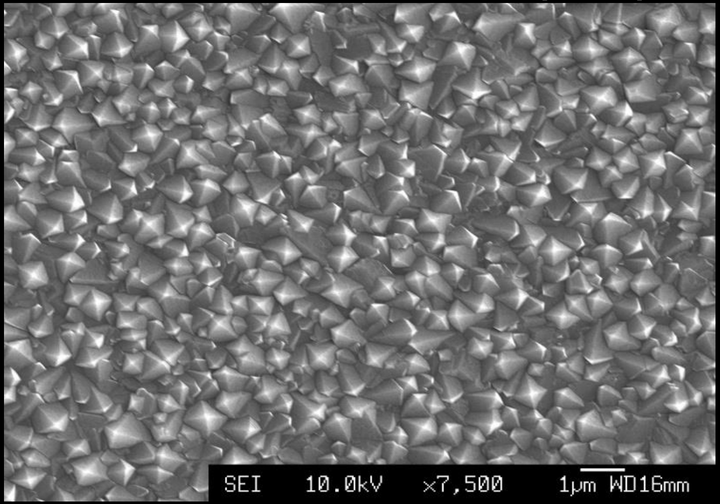


CVD Diamond

- Material Requirements for Thermionic Diamond
  - Low Work Function surfaces with Stable Negative Electron Affinity
  - High Electrical Conductivity using efficiently doped n-type layers



Emitter Surface - C(100)



Collector surface – C(111)

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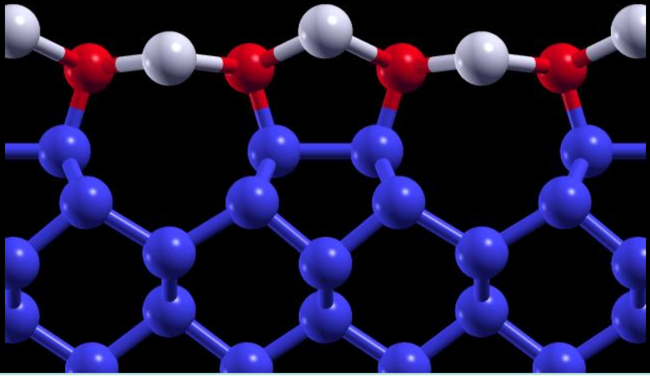
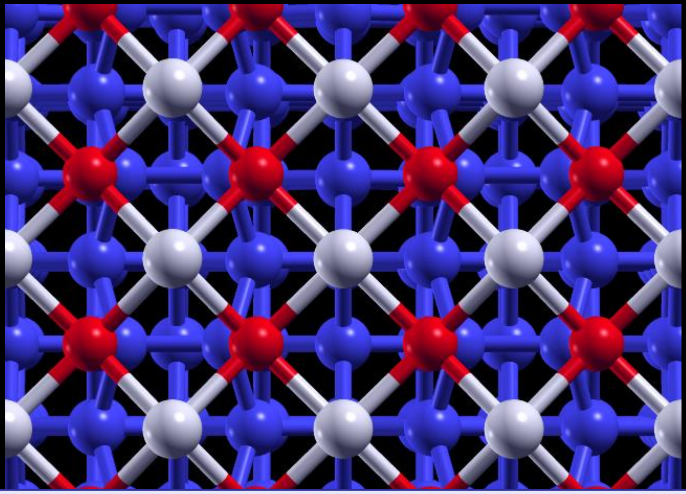
Diamond Surface Studies - Modelling

- Oxygen forms stronger bonds with Li than C does. On the other hand, O-terminated surfaces have a very high PEA (high negative surface charge due to lone pairs).



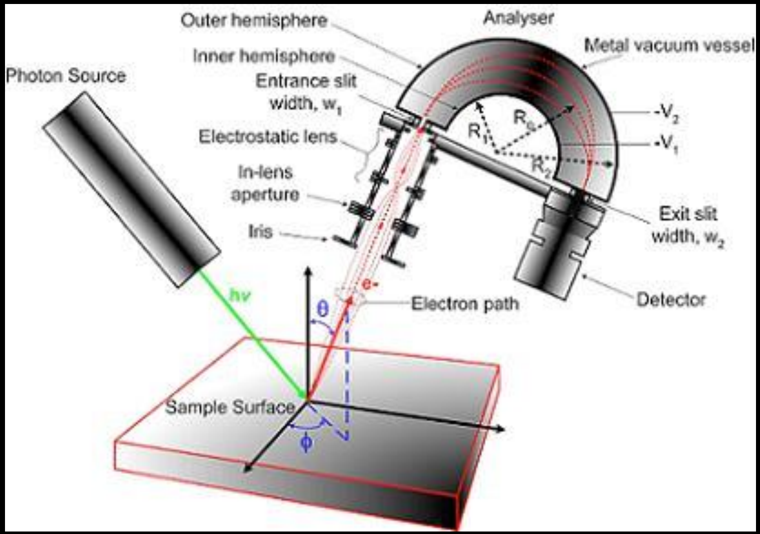
In the optimal structure, the Li-O displacement vectors are almost oriented parallel to the surface, not perpendicular as required for a traditional dipole.



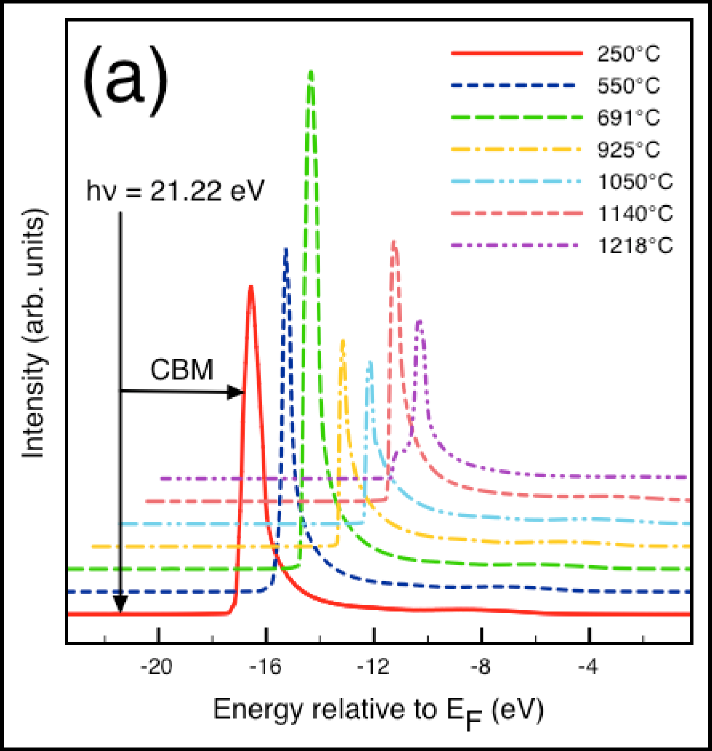
Calculated dipole is large – the NEA is more than twice that of the hydrogenated surface at -4.5 eV.

K.M. O'Donnell et.al.,Phys.Rev.B 82, 115303 (2010)

UV Photoelectron Spectroscopy of SC diamond, B-doped C(100):O,Li



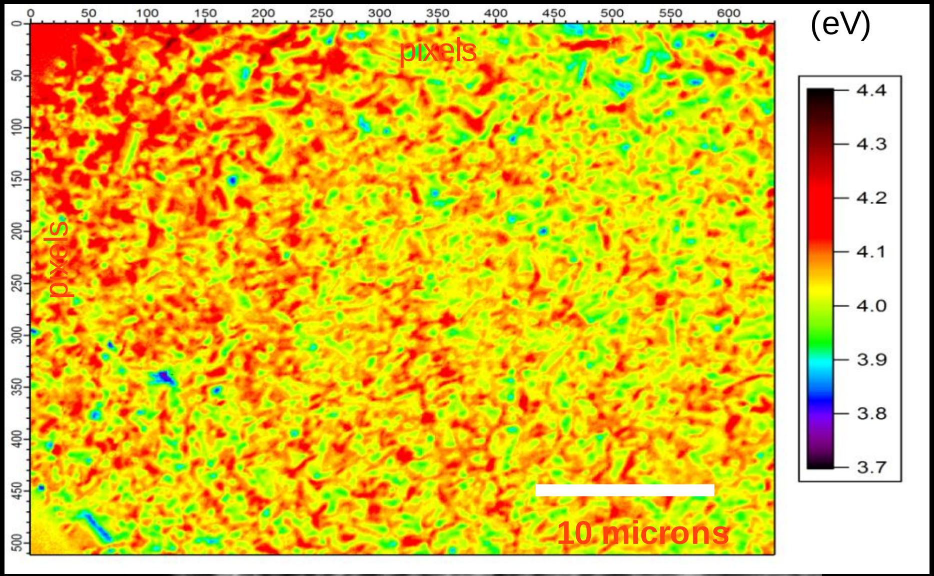
UPS: large NEA peak, remains even after annealing at 1000°C. Some breakdown is evident above1200°C.

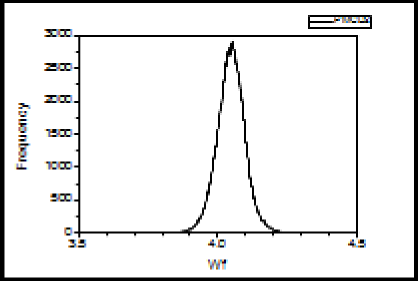


'Photoelectron emission from lithiated diamond', K. M O'Donnell, T.L Martin, M.T Edmonds, A.Tadich, L.Thomsen, J. Ristein, C.I Pakes, N. A Fox, L. Ley, Physica Status Solidi (a), 2014. DOI 10.1002/pssa.201431414

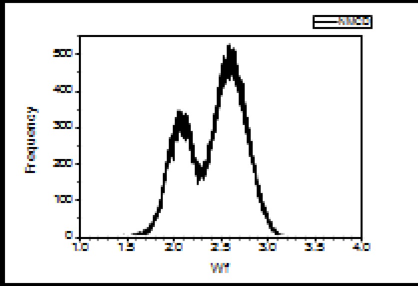
Work function of CVD Diamond films

- NanoESCA shows the average photo-electric work function of boron-doped , p-type diamond is ~4.05eV
- For nitrogen doped, n-type (1.7eV level) ranges from 2.0eV to 2.8eV
- Thermionic emission will be insignificant at temperatures accessible to solar heating (mA/cm^2 instead of A/cm^2)
- How can net flux of emission current be increased?





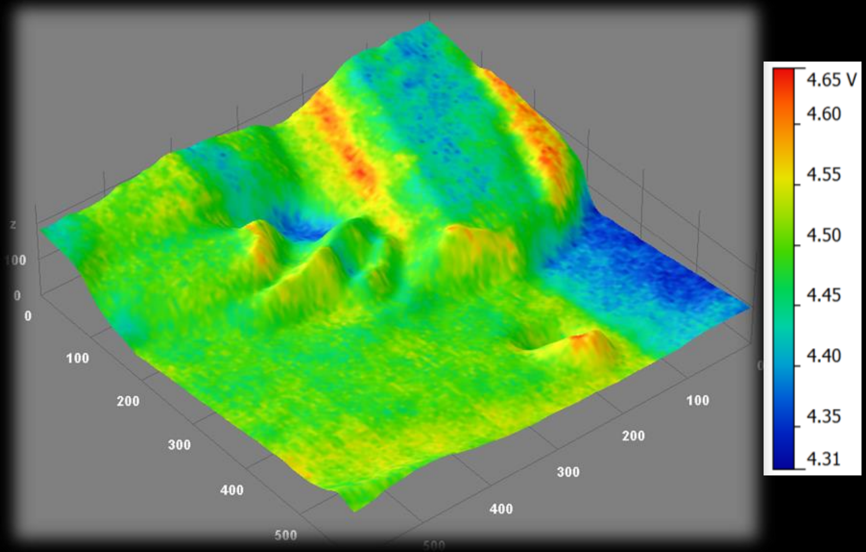
p-type



n-type

Use of energy-filtered photoelectron emission microscopy and Kelvin probe force microscopy to visualise work function changes on diamond thin films terminated with oxygen and lithium mono-layers for thermionic energy conversion', *N. A.Fox, et.al., Int. J. Nanotechnol., Vol. 11, Nos. 9/10/11, 2014.*

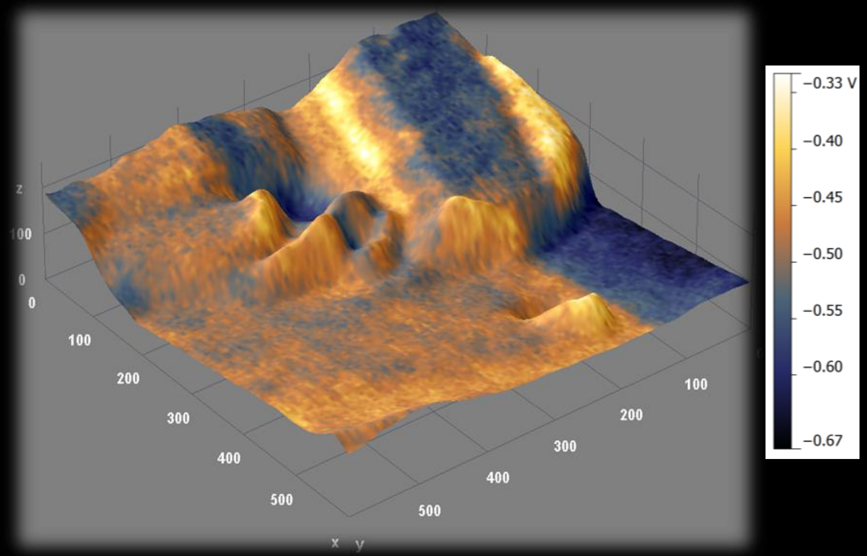
UHV Scanning Kelvin Probe Microscopy



Work function values of boron doped diamond with Li-O surface termination superimposed onto a surface plot of the same area

- Possible to see work function differences between crystals

- Negative Electron Affinity: vacuum level under conduction band



Negative Electron Affinity values of boron doped diamond with Li-O surface termination superimposed onto a surface plot of the same area

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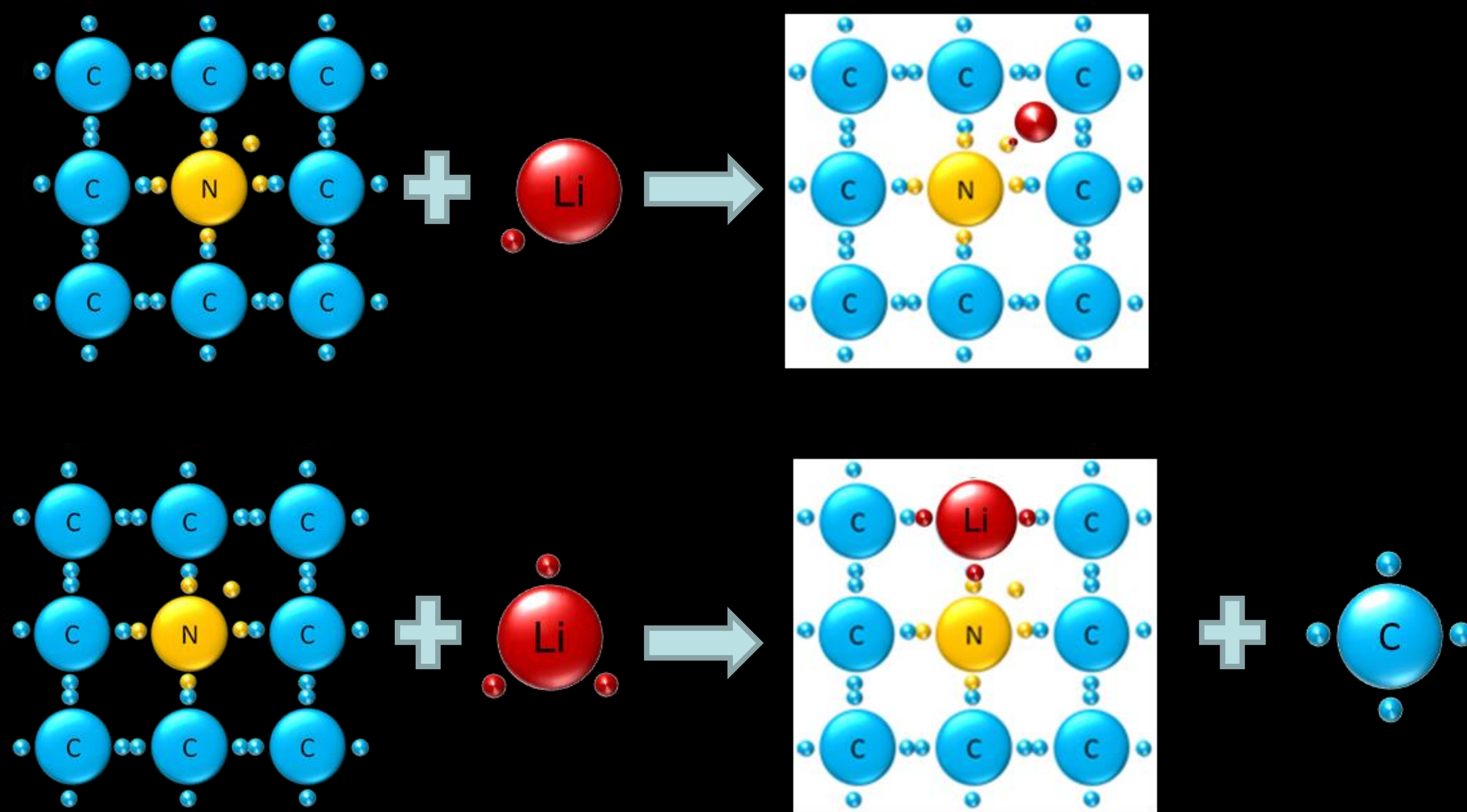
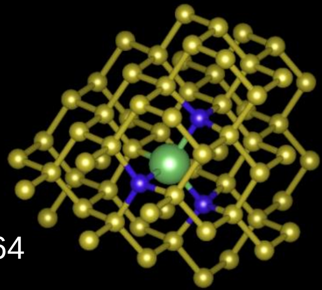
Modelling Co-doped Diamond



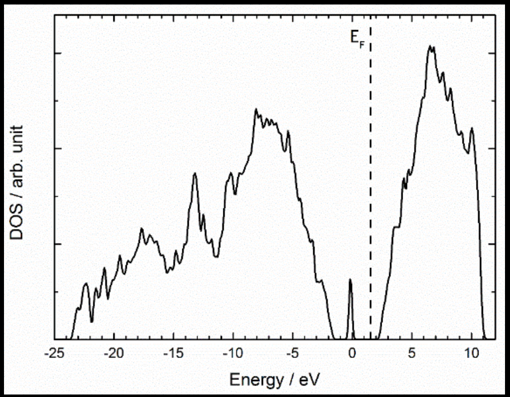
Li-N co-doped diamond films - CASTEP code simulations

Substitutional defect

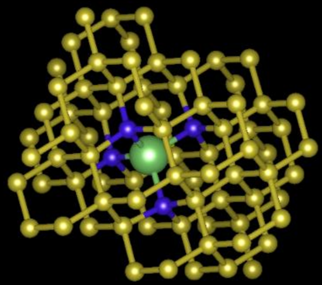
1:3 Li-to-N ratio



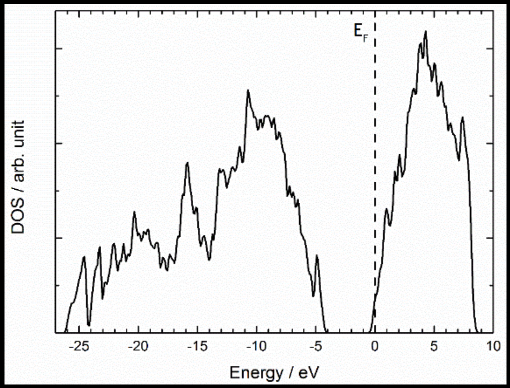
- Formation Energy: 3.88 eV
- Dopant concentration
  - 1.56% for Li (1 atom of Li in 64 atom supercell)
  - 4.69% for N (3 atoms of N in a 64 atom supercell)
- Fermi Level (E_F) 0.5 eV below E_c.
- Dopant level 1.90 eV below E_c.



1:4 Li-to-N ratio

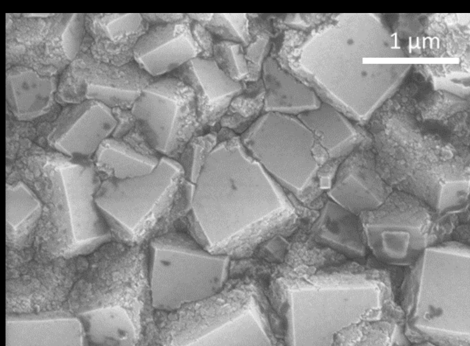


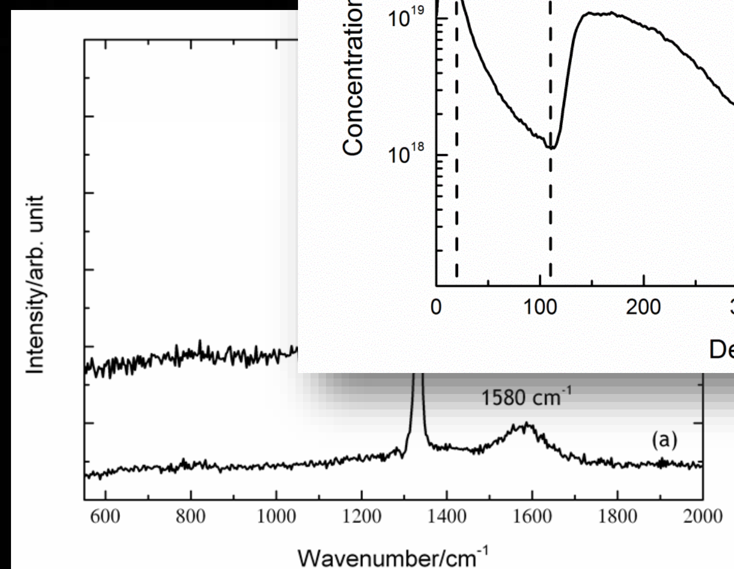
- Formation Energy: 4.88 eV
- Dopant concentration
  - 1.56% for Li (1 atom of Li in 64 atom supercell)
  - 6.25% for N (4 atoms of N in a 64 atom supercell)
- Fermi Level (E_F) <0.1 eV below E_c.
- Dopant level – <0.1 eV below E_c.
- The E_F and dopant energy level lying within and just below the conduction band.

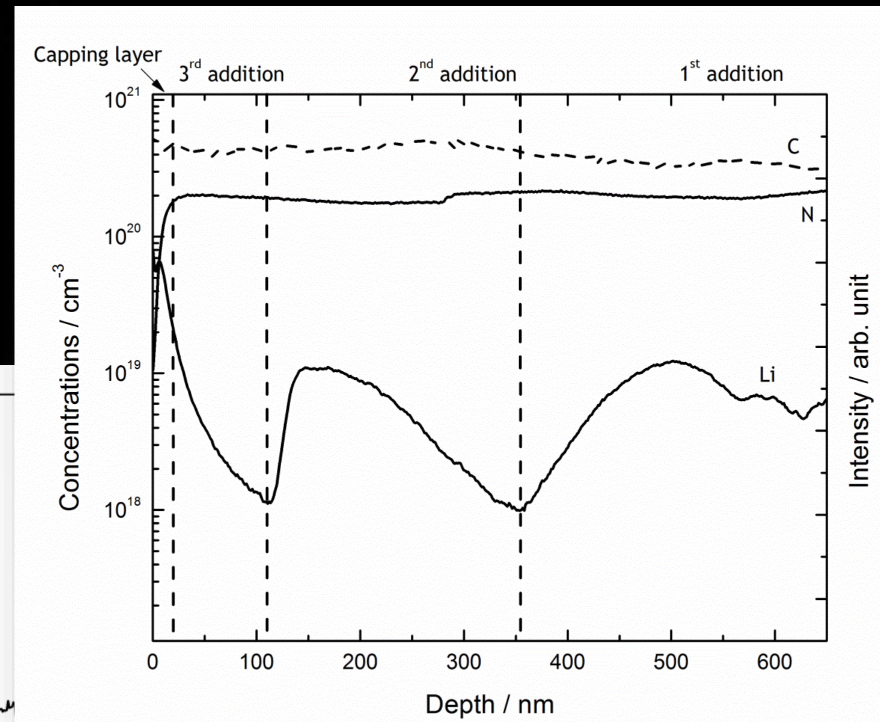


Li-N co-doped diamond films - Hot Filament CVD

- ~1.1×10^{19} atoms of Li/cm^{-3}
- ~2.1×10^{20} atoms of N/cm^{-3}
- Li:N – 1:19
- Properties dominated by N atoms





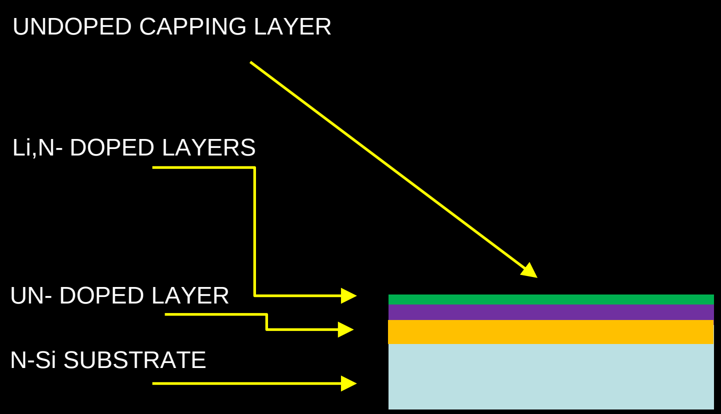


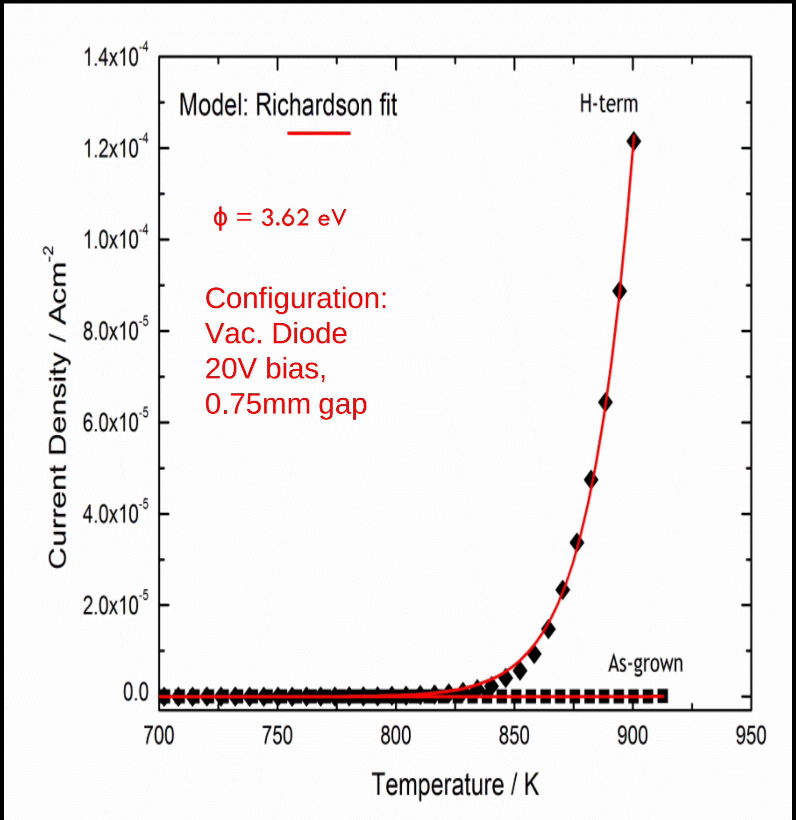
M. Z.Othman, P.W.May, N.A.Fox,P. J. Heard, Diamond & Related Materials 44 (2014) 1–7.

Li-N (1:19) co-doped diamond films - Thermionic Emission

Co-doped active layer:

- Microcrystalline CVD diamond
- Hydrogen-terminated surface





Measurements taken at ASU 2013

- $T_{threshold}$ = 800 K
- T_{max} = 900 K

R. J. Nemanich, F. A.M. Koeck. Tianyin Sun, & Z.Othman

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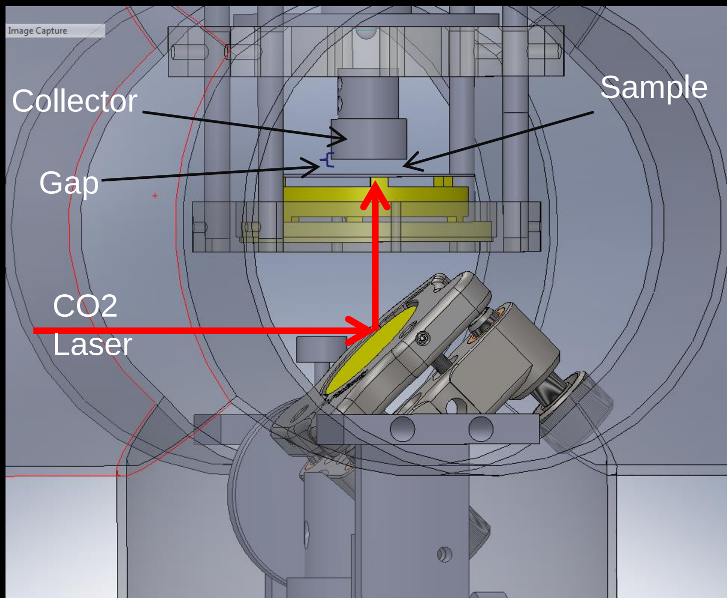
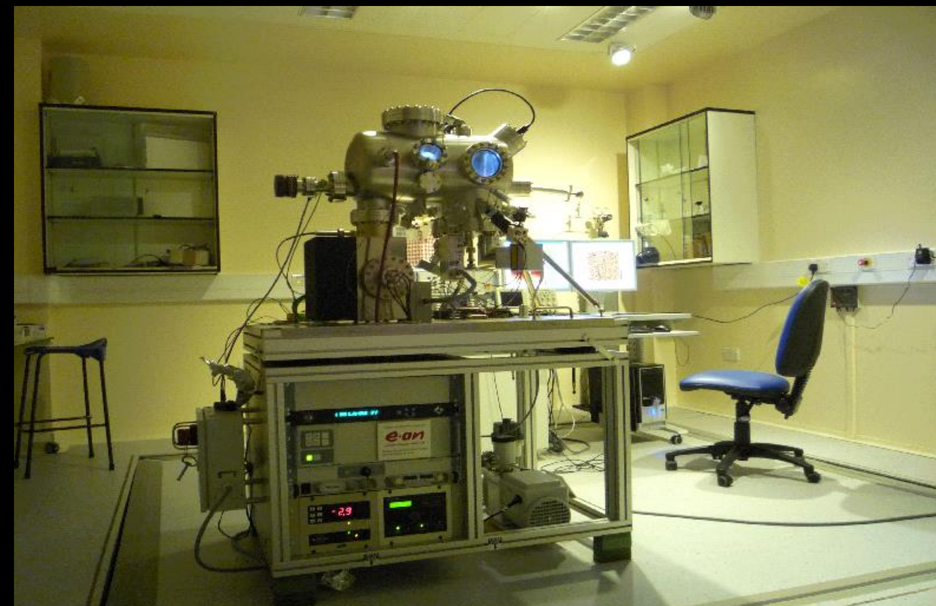
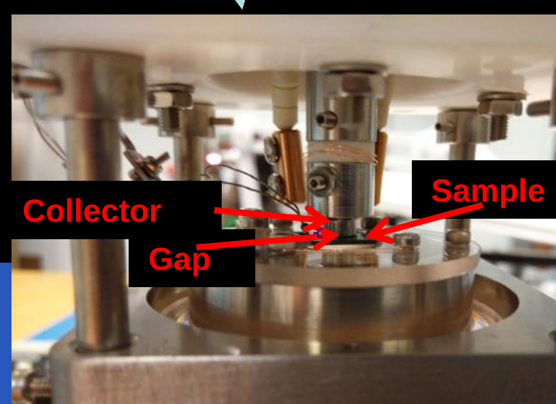
DTC Test Rigs



Laser-heated
Thermionic Set-up



NSQI- Ultra-quiet Laboratory UHV SPM
with Radiative heating



DTC Test Rigs

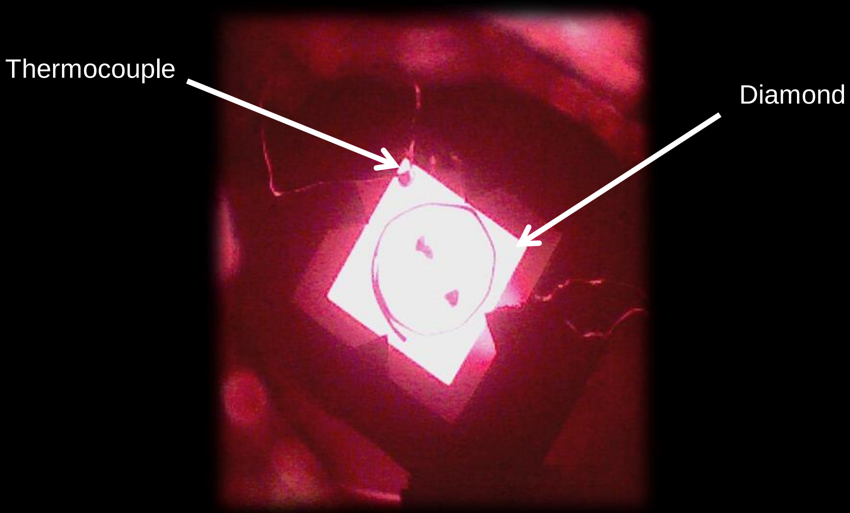
Electrically-heated
Thermionic Set-up

Solar
TDC Test Rig

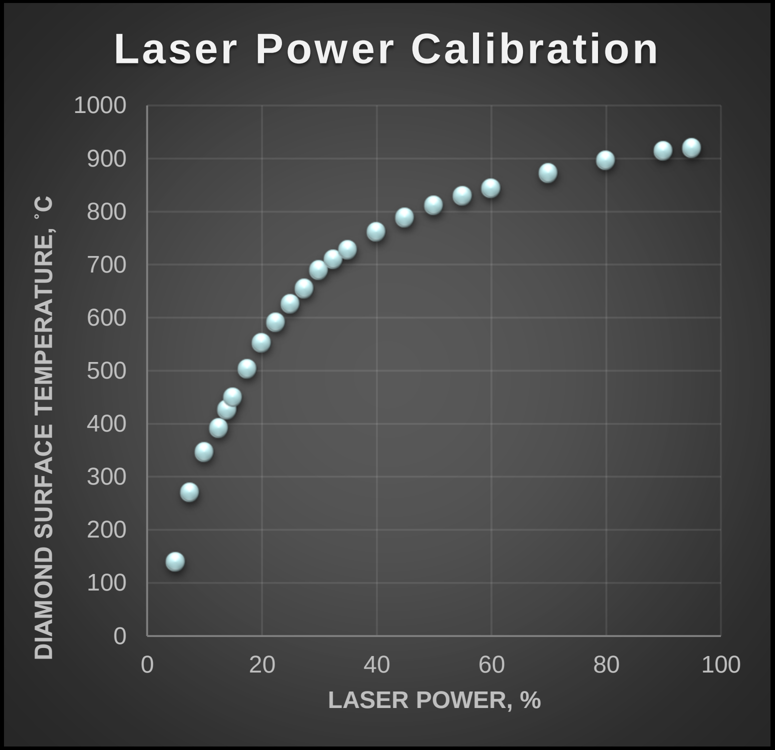
Laser-heated Temperature Calibration

Two temperature measurement methods:

- Two colour Pyrometer – High temp range
- Thermocouple : – Low temp range



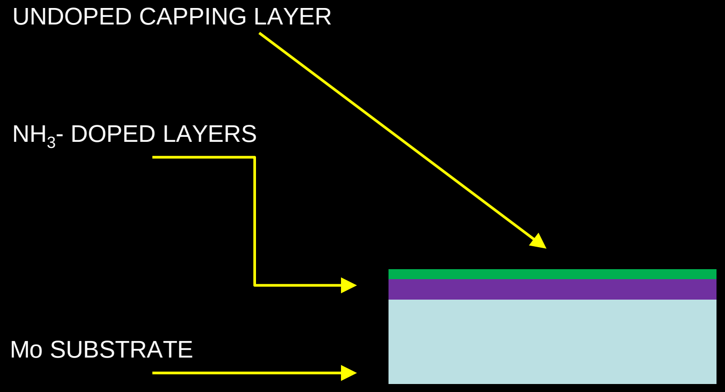
Heating test of free-standing doped diamond

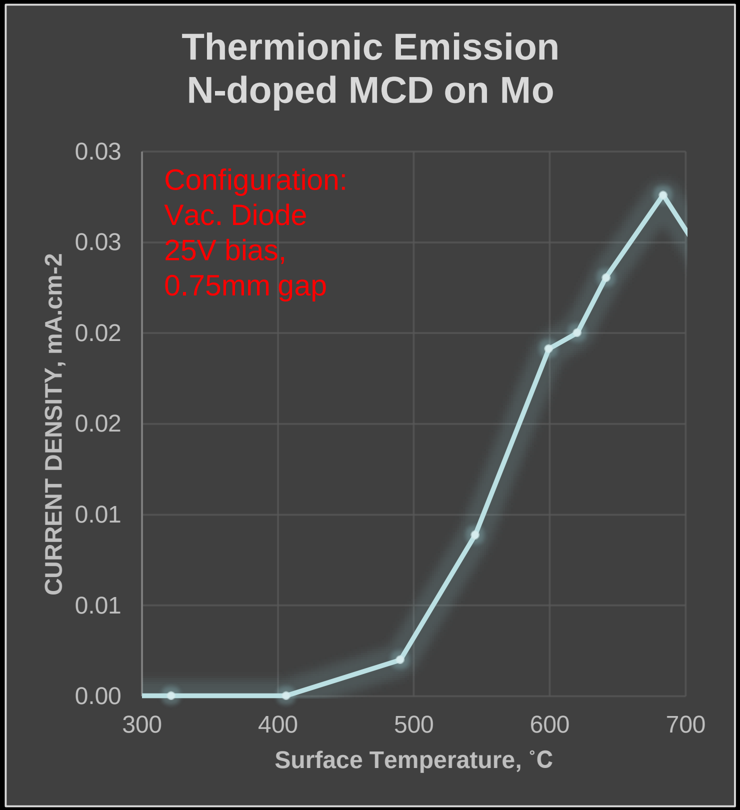


Laser-heated TE - Preliminary Results

Single elemental dopant:

- Microcrystalline CVD Diamond (MCD)
- Metal Substrate
- Hydrogen-terminated surface
- N content ~1 x 10^{20} atoms.cm^{-3}



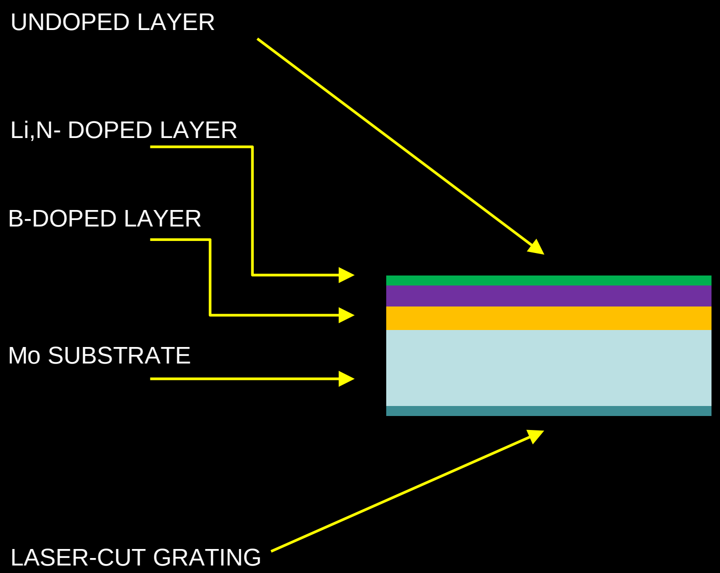


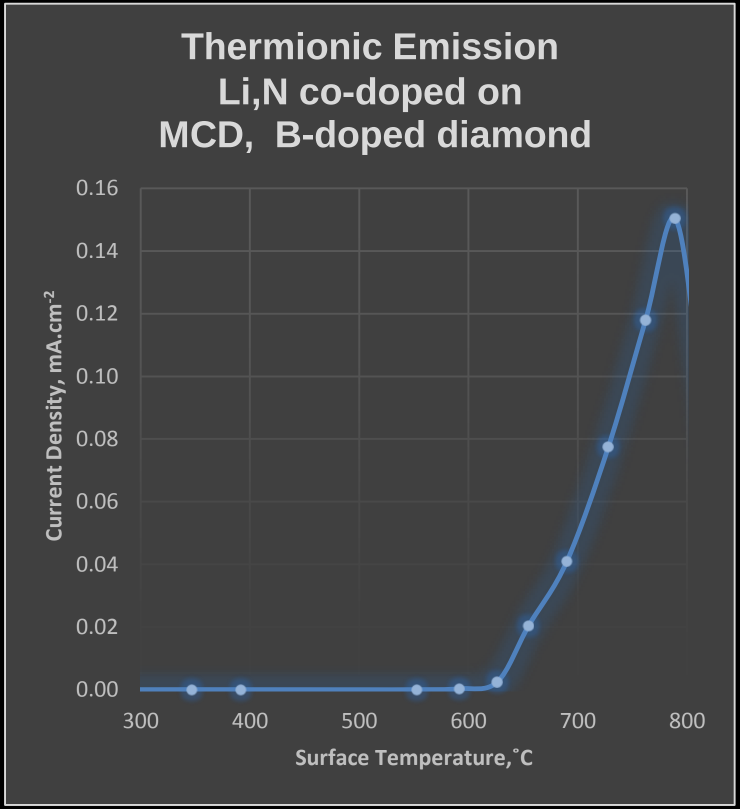
- $T_{threshold}$ = 673 K
- T_{max} = 963 K

Laser-heated TE - Preliminary Results

Co-doped active layer:

- Metal substrate
- Hydrogen-terminated surface
- Li:B ratio TBD



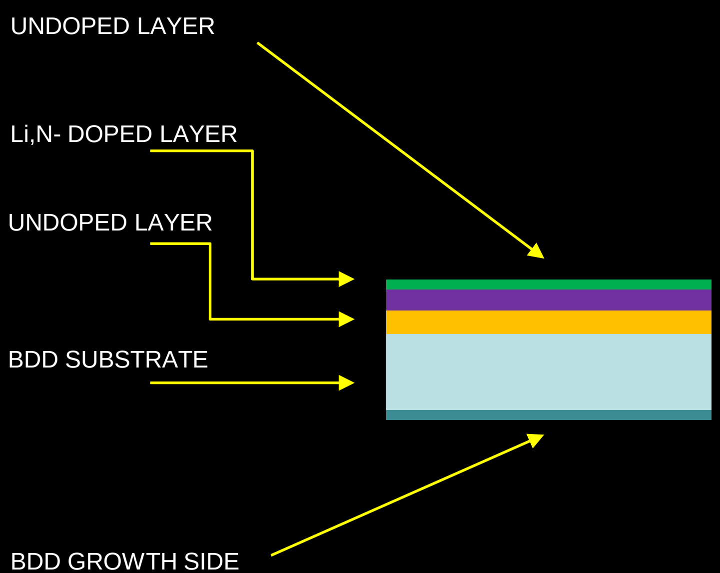


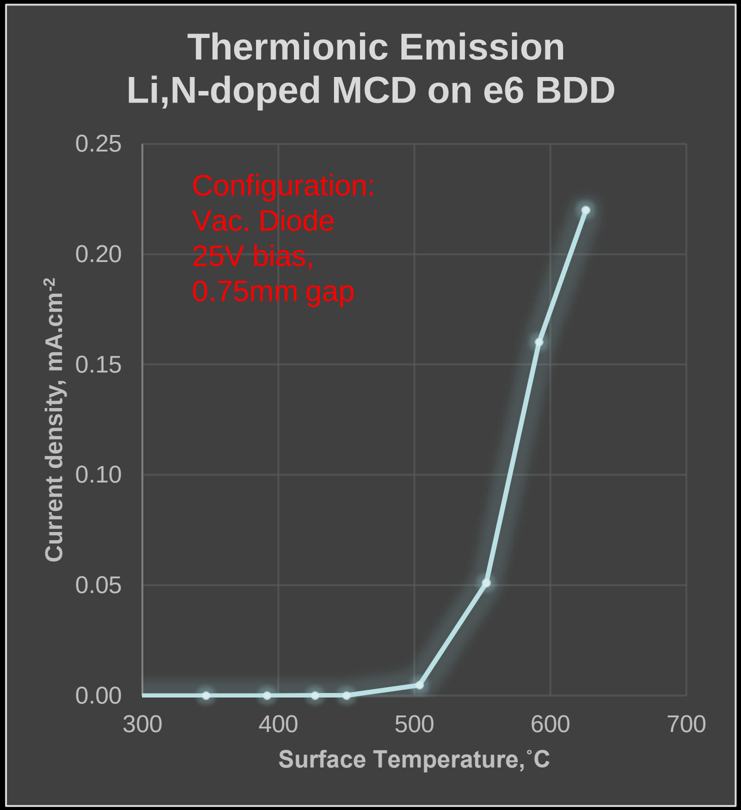
- $T_{threshold}$ = 903 K
- T_{max} = 1063 K

Laser-heated TE - Preliminary Results

Co-doped active layer:

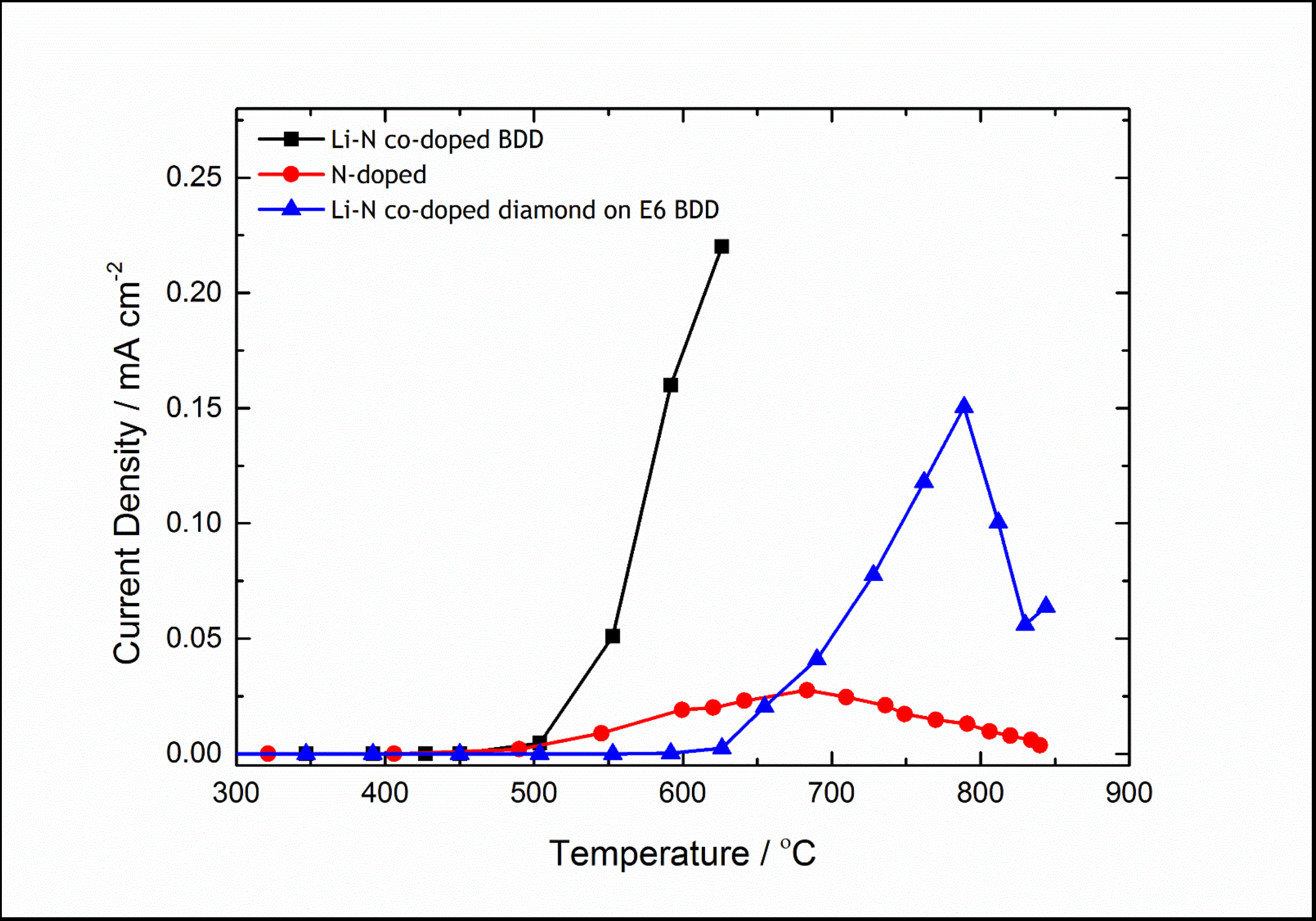
- Free-standing e6 BDD substrate
- Hydrogen-terminated surface
- Li:N ratio 1:19





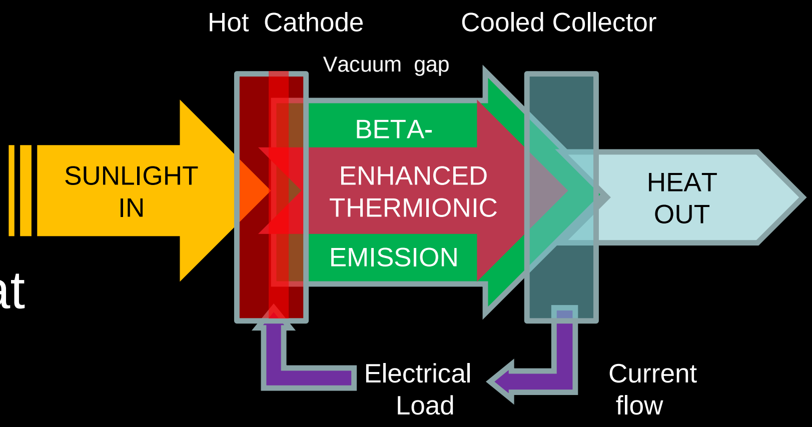
- $T_{threshold} = 723$ K
- $T_{max} = 899$ K

Laser-heated TE - Summary



Isotopic Diamond Converters

- Use of ^{13}C & ^{12}C diamond
  - Thermal carrier confinement
- Use of ionising ^{14}C diamond
  - Generates e-h pairs in bulk
  - Potential to generate high SEE at a diamond surface
- Potential outcomes
  - Increased flux of thermionic carriers leaving hot cathode
  - New electrode architectures



Acknowledgements

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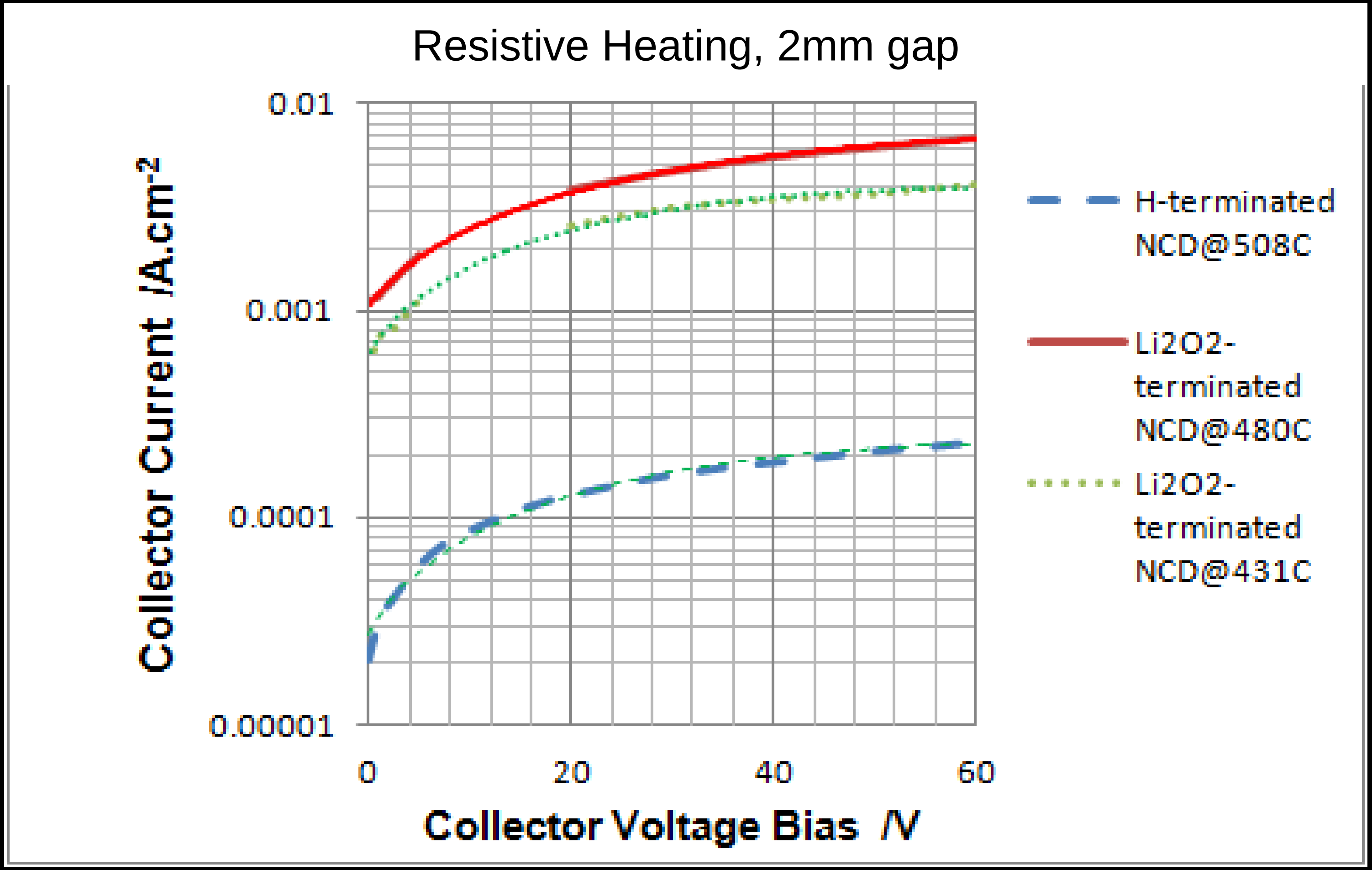
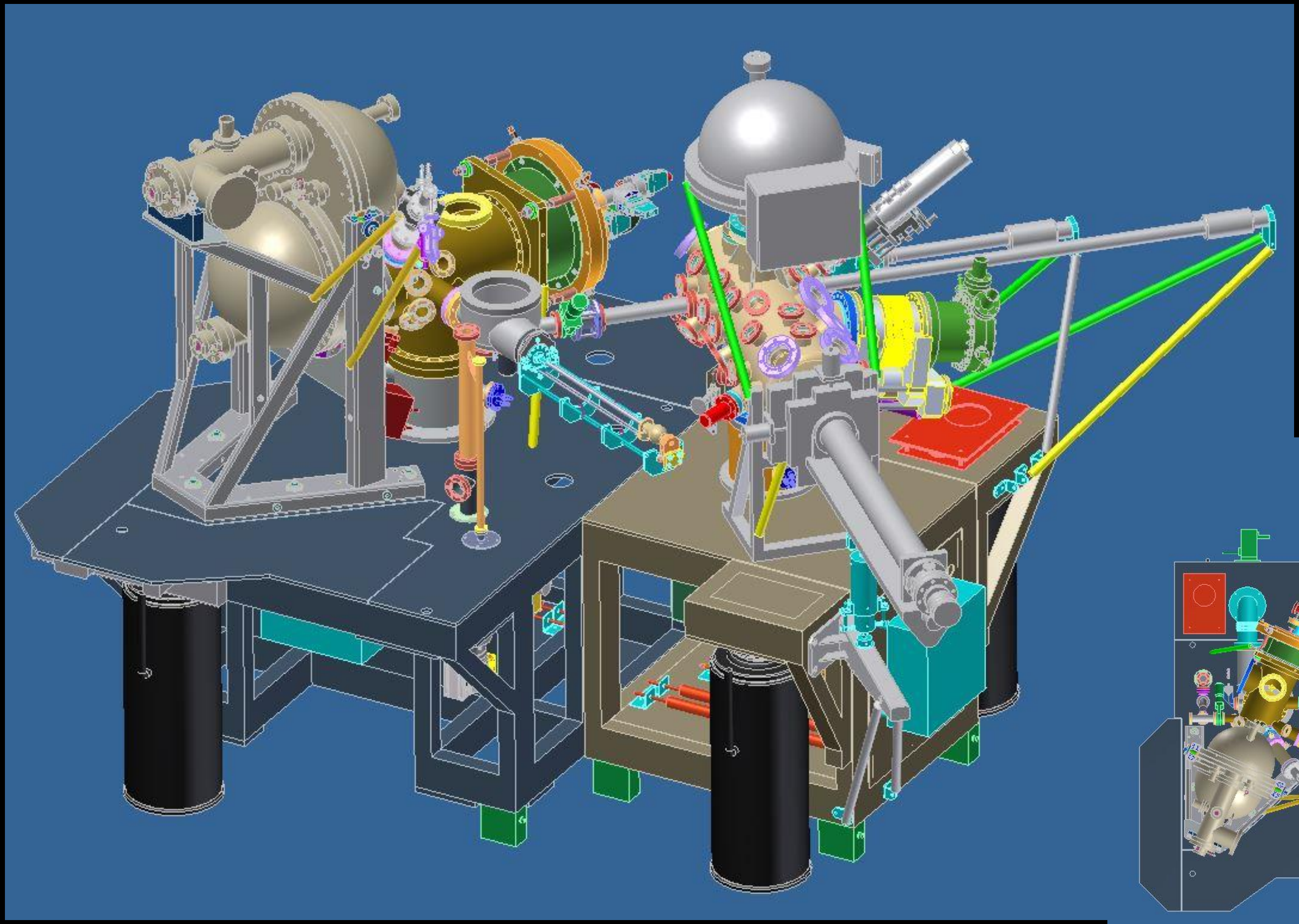
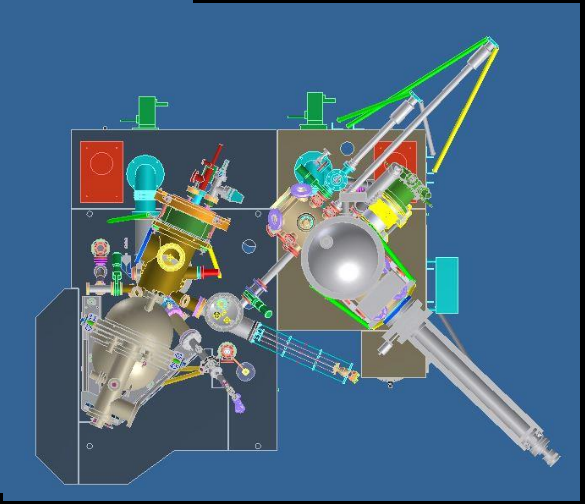
- ASU:
  - R. J. Nemanich, F. A.M. Koeck. Tianyin Sun
- MINATEC-LETI:
  - Olivier Renault

Li-N co-doped diamond films + O,Li termination - Thermionic Emission



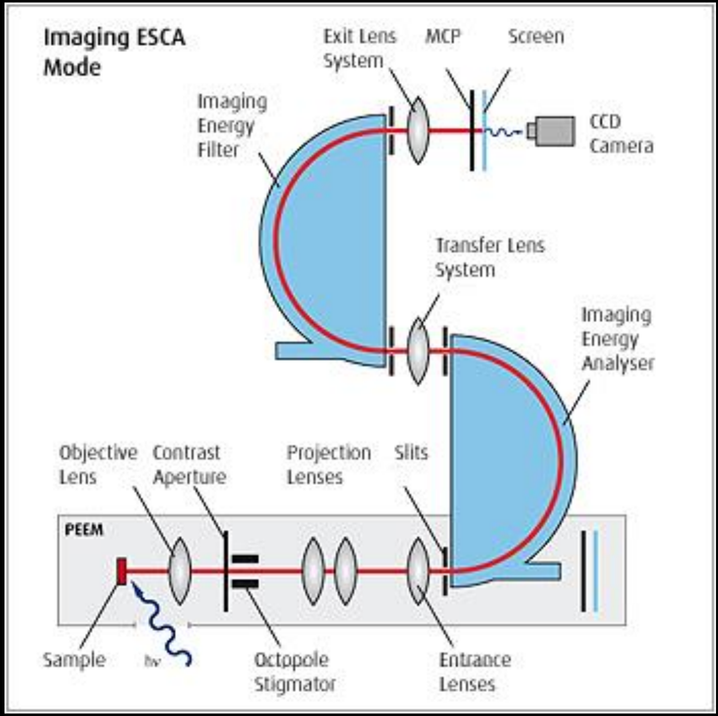
Mk II system configuration for Bristol





NanoESCA Laboratory Specification

- Focussed Light sources
  - Energy Resolution in PEEM modes
    - VUV : 50 (28) meV
    - X-ray : 190 (100) meV
  - Lateral edge resolution in PEEM
    - VUV: 60 (20) nm
    - X-ray : 480 (320) nm
- Switchable between real space and k-space modes by control of transfer lens (k space resolution 10Å^{-1})

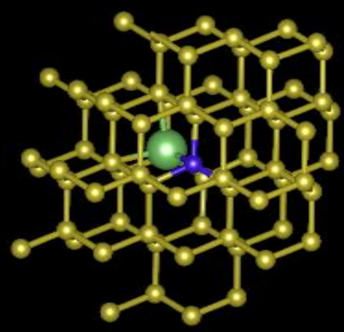


Li-N co-doped diamond films - CASTEP code simulations

Interstitial defect

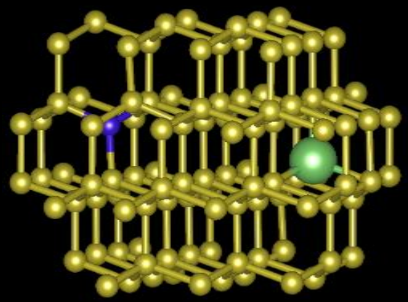
1:1 Li-to-N ratio (next to each other)

- Formation Energy – 9.41 eV
- Dopant concentration
  - 1.56% for Li (1 atom of Li in 64 atoms supercell)
  - 1.56% for N (1 atoms of N in 64 atoms supercell)



1:1 Li-to-N ratio (far apart)

- Formation Energy – 11.32 eV
- Dopant concentration
  - 1.56% for Li (1 atom of Li in 64 atoms supercell)
  - 1.56% for N (1 atoms of N in 64 atoms supercell)



- From the formation energy calculated. N atom act as a trap to pin down Li atom and this reduced the mobility of Li in diamond at high temperature.
- This concept is suitable to immobilise Li in diamond lattice.