Analysis of Thermoradiative Thermal Energy Conversion

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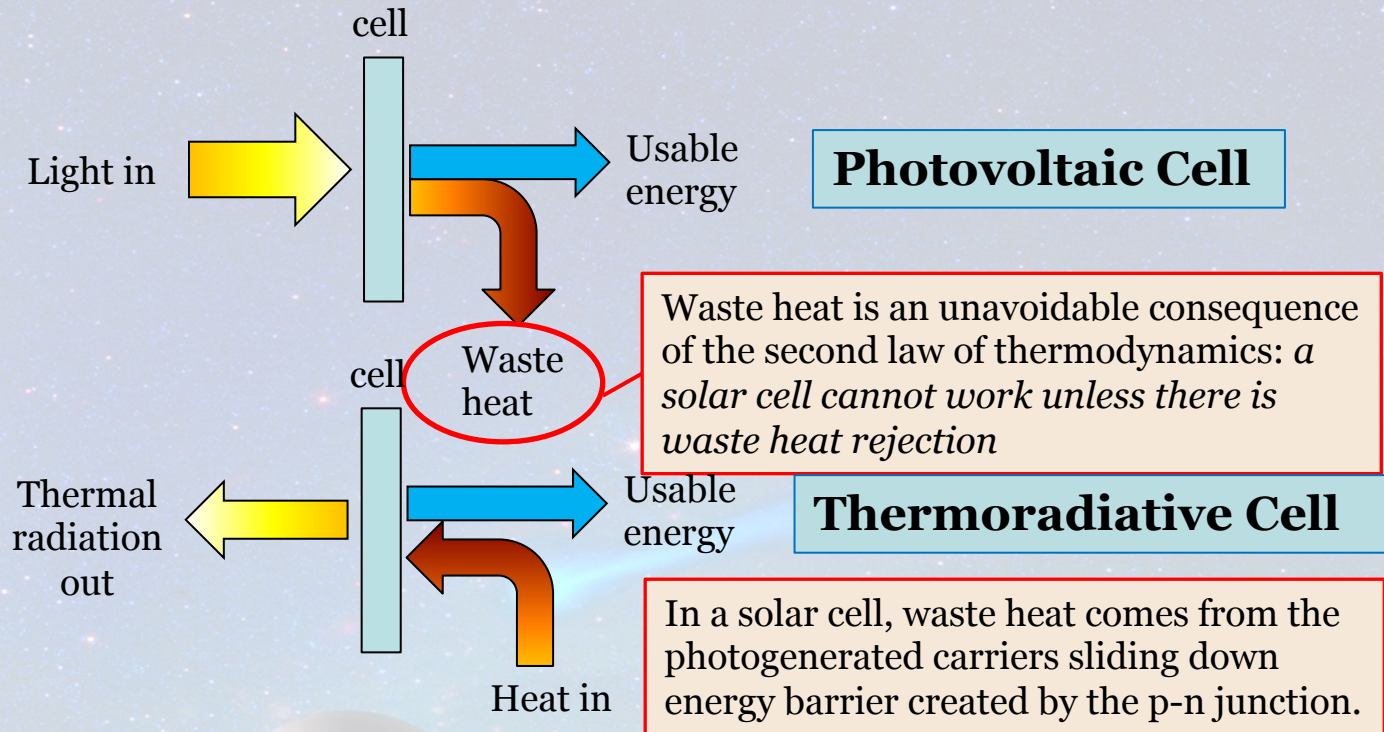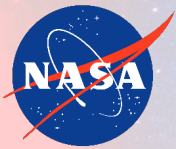NASA John H. Glenn Research Center

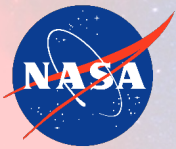# What is a Thermoradiative cell?
And why should we care?

- A thermoradiative cell is a new method for converting heat energy into electrical power
  - First detailed by Strandberg in 2015 and by Santhanam and Fan in 2016 (based on concepts elucidated by Byrnes, Blanchard, and Capasso)
  - Operationally similar to a photovoltaic cell, but thermodynamically exactly backwards

- No moving parts

- Think of it as a panel that acts like a **thermal radiator that generates power**
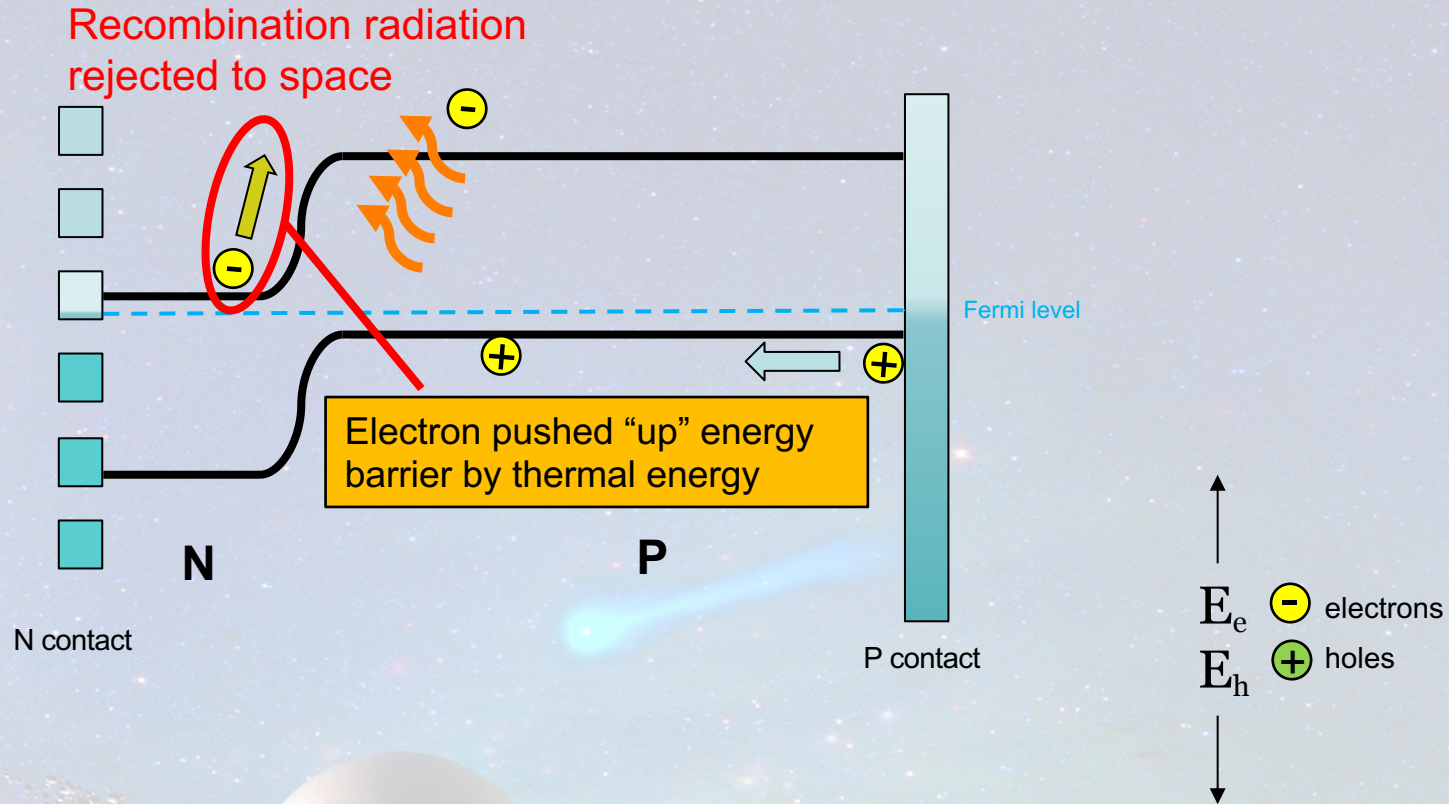
Photovoltaic Cell vs Thermoradiative Cell

cell

Light in → → Usable energy

Photovoltaic Cell

Waste heat

Waste heat is an unavoidable consequence of the second law of thermodynamics: *a solar cell cannot work unless there is waste heat rejection*

cell

Thermal radiation out ←

← Usable energy

Thermoradiative Cell

Heat in

In a solar cell, waste heat comes from the photogenerated carriers sliding down energy barrier created by the p-n junction.

Operation of thermoradiative cell: band diagram

Recombination radiation rejected to space

Electron pushed "up" energy barrier by thermal energy

Fermi level

N

P

N contact

P contact

E_e — electrons

E_h — holes

Deep space (~10 K)

heat in

light out

Fermi level

N

P

N contact
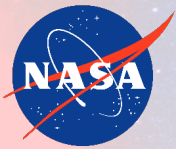
P contact
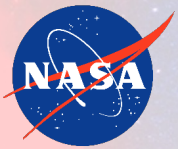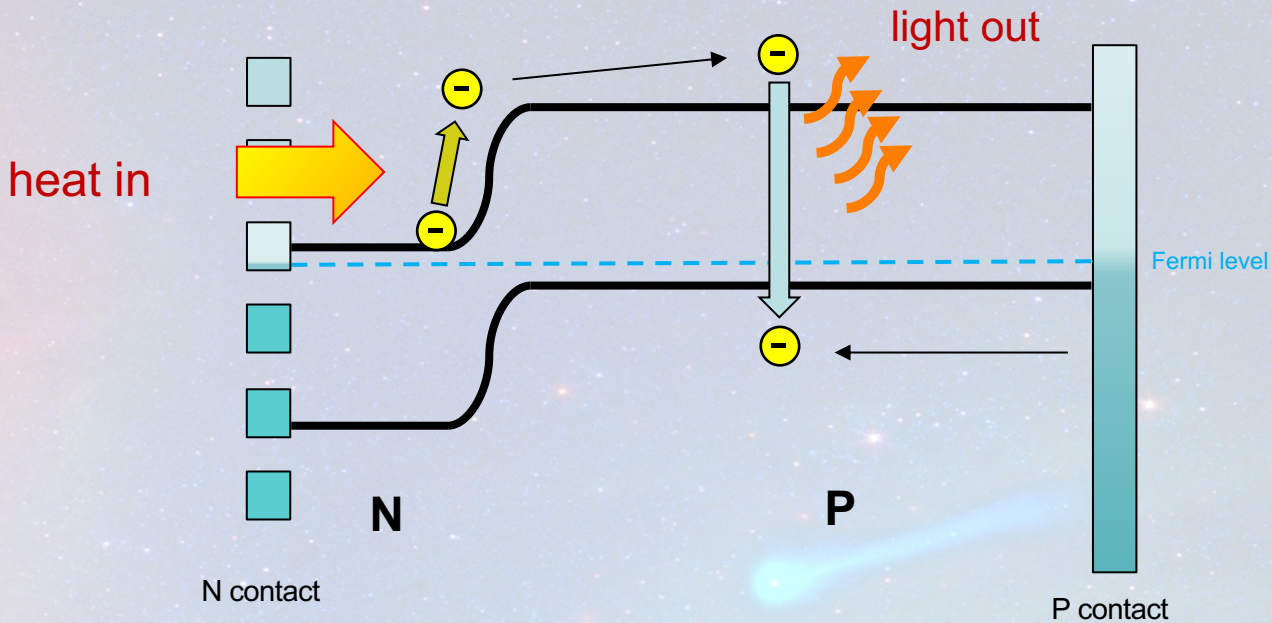
Terrestrial Applications?

- Thermoradiative conversion could, in principle, be used for energy conversion for any thermal source.

- The original proposals were for terrestrial applications. However, the Earth's atmosphere is not IR transparent, and so effective temperature of the heat sink is at best 200K (for a clear night sky with low humidity), and in most applications much higher.

- This results in a downward infrared flux which cancels out part of the upward radiation driving the cell current
  - Earth also has a surface environment in which convective cooling competes with radiative cooling for heat transfer.
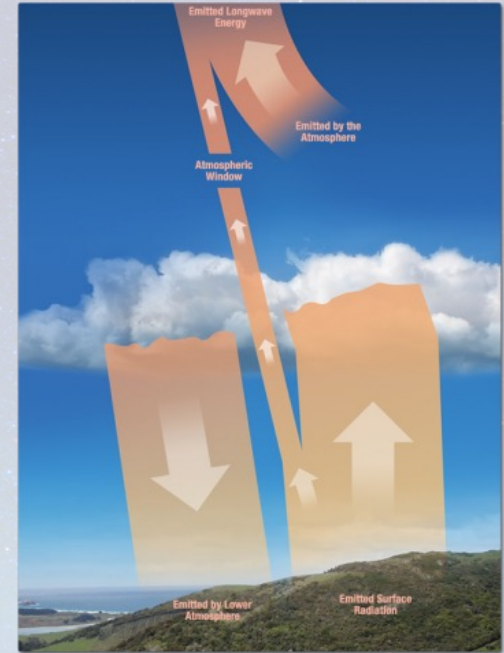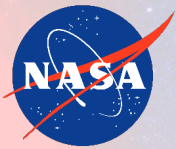

Upwelling and downwelling IR flux in Earth's atmosphere
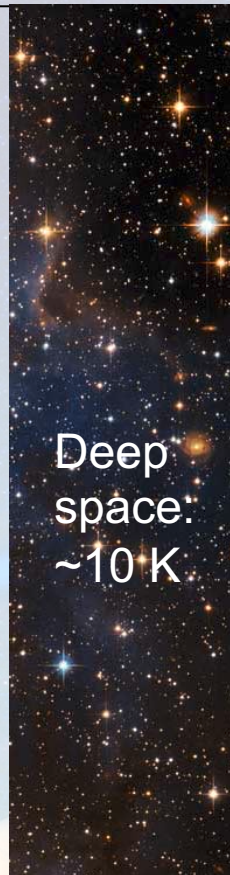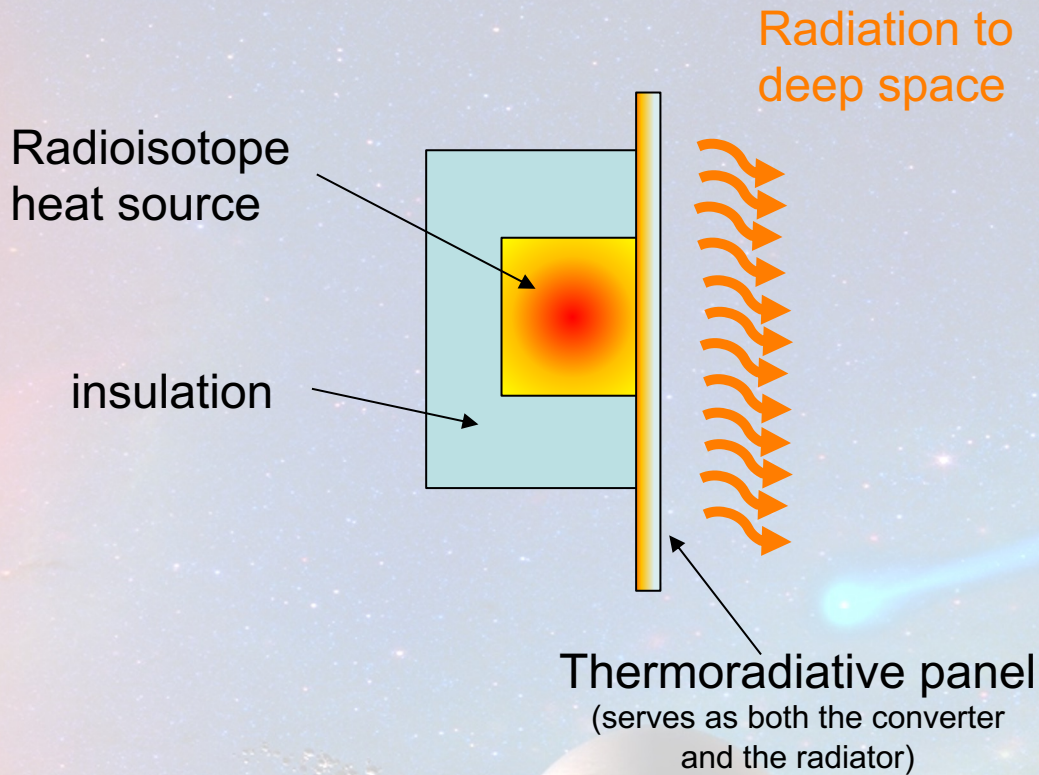
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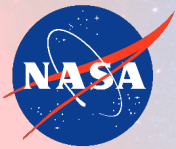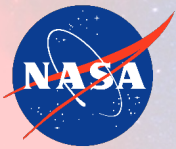
Space Applications

- In-space applications are well suited for this technology, since with no atmosphere the cell radiates to the heat sink of deep space. Heat source would be a radioisotope (*e.g.*, Pu-238) or nuclear reactor.
  - Temperature of deep space is often quoted at 4K, but inside the solar system, actual effective temperature ~10-12K
  - However, in practice the difference here is unimportant, since even 12K is << operating temperature of a realistic heat source, and can be ignored

- Planetary bodies with atmospheres (Venus, Mars, Titan) not ideal.
  - Atmospheric convection will be significant heat loss.
  - Infrared opacity of the atmospheres means that the cold side temperature will be the atmospheric temperature, not the temperature of deep space.

- For bodies with no atmosphere (*e.g.*, moon), radiating surface must be in the dark & shielded from other sources of infrared, such as the Earth, and the hot lunar surface.

Conceptual operation of thermoradiative cell in space

Radiation to deep space

Radioisotope heat source

insulation

Thermoradiative panel
(serves as both the converter
and the radiator)

Deep space: ~10 K

*The effective temperature of deep space is only 4K if you are outside the galaxy. Inside the solar system zodiacal light makes the effective temperature more like 10-12K

- Solar cells need to be made from semiconductors with bandgap comparable to the peak output of the solar spectrum
  - Solar peak is ~0.5 to 1 micron, so optimum bandgap is order of 1-2 eV

- Thermoradiative cells need semiconductor bandgap comparable to the wavelength of the thermal spectrum
  - Thermal peak for ~600K emission is around ~6 micron, so optimum bandgap is ~ 0.1-0.2 eV
    - (back of the envelope)
  - Thus: **Narrow bandgap semiconductors**
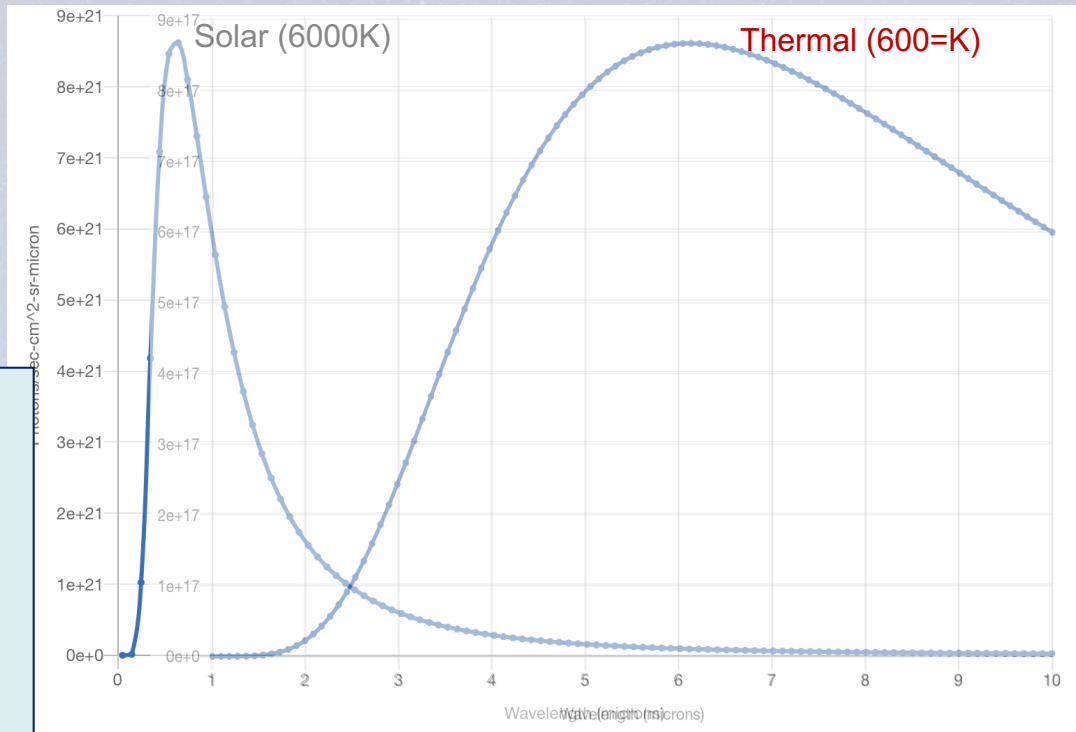
Einstein's relation: $E = hc/\lambda$

III-V semiconductors

Energy Gap and Lattice...

Optimum semiconductors for solar cells are here
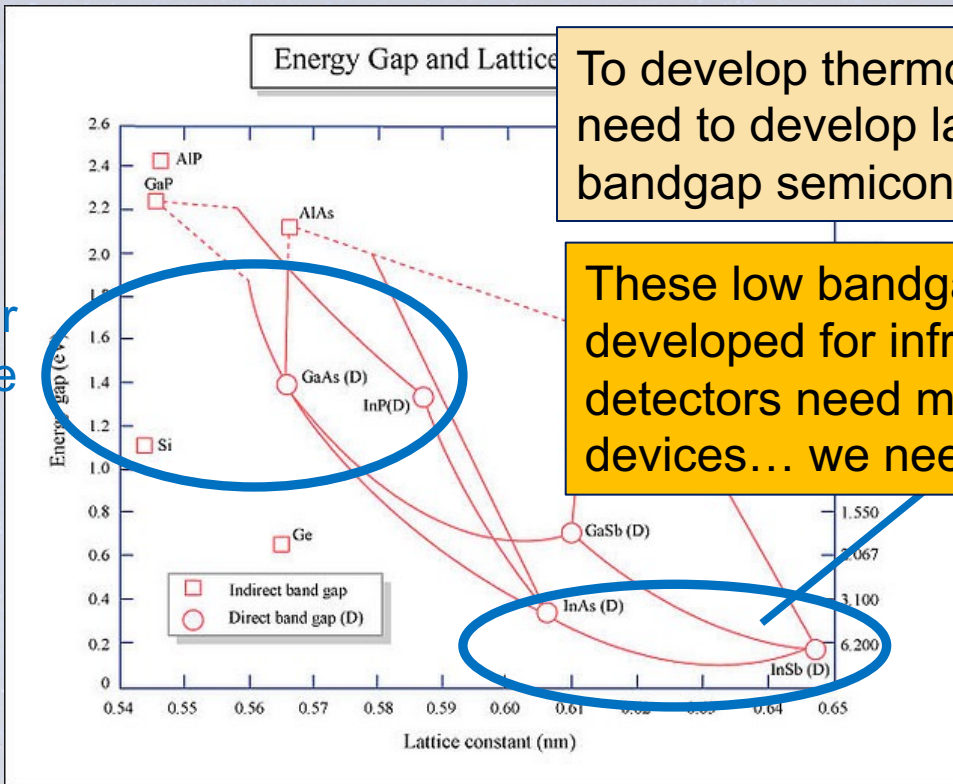
To develop thermoradiative cells, we need to develop large-area, low bandgap semiconductors

These low bandgap materials are being developed for infrared detectors, but IR detectors need millimeter scale devices… we need square meters

...thermoradiative cells are down here

Carnot Efficiency

- As will all heat engines (including solar cells), a thermoradiative cell is limited to a maximum possible efficiency by the Carnot efficiency limit,

$$\eta_{carnot} = (1 - T_c/T_h)$$

where T_h is the (absolute) operating temperature of the cell and T_c is the (absolute) temperature of the heat sink,

- However, in the real world, cells are not likely to approach the Carnot efficiency limit.

Theoretical Current

- Short circuit current is the dark current I_o, which in general is a function of the semiconductor parameters (bandgap, lifetime, diffusivity, *etc.*)

- To make a device-independent model of the maximum current, note that in the ideal case each carrier in the generated current releases exactly one photon of recombination radiation. The maximum possible current I_o is thus qN, where N is the number of photons emitted.

- But the thermally-generated radiation is limited by thermodynamics, and cannot be greater than the blackbody radiation.

  – In the ideal case, the outgoing radiation is thus the Planck spectrum, with emissivity of 1 for photon energy greater than the bandgap, and emissivity of 0 for energy less than the bandgap.

- Current can be calculated by integrating the blackbody spectrum, expressed as number of photons, from E_g to ∞ (λ=0 to λ_c)

$$N(\text{per unit area}) = \int (8\pi E^2/h^3c^3)(e^{E/(kT)}-1)^{-1}$$

- **Note that this is the same as the I_{sc} of an (ideal) thermophotovoltaic cell of the same bandgap operating at the same temperature.**
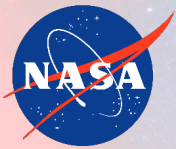
Power as a function of temperature

- Since the number of photons in the blackbody spectrum is proportional to temperature cubed, and the voltage at the maximum power point is directly proportional to temperature, the total power output is proportional to T^4.

> Thus, although the efficiency has only a small temperature dependence*, the power output depends strongly on temperature.

*assuming that the environmental temperature is much less than the device temperature
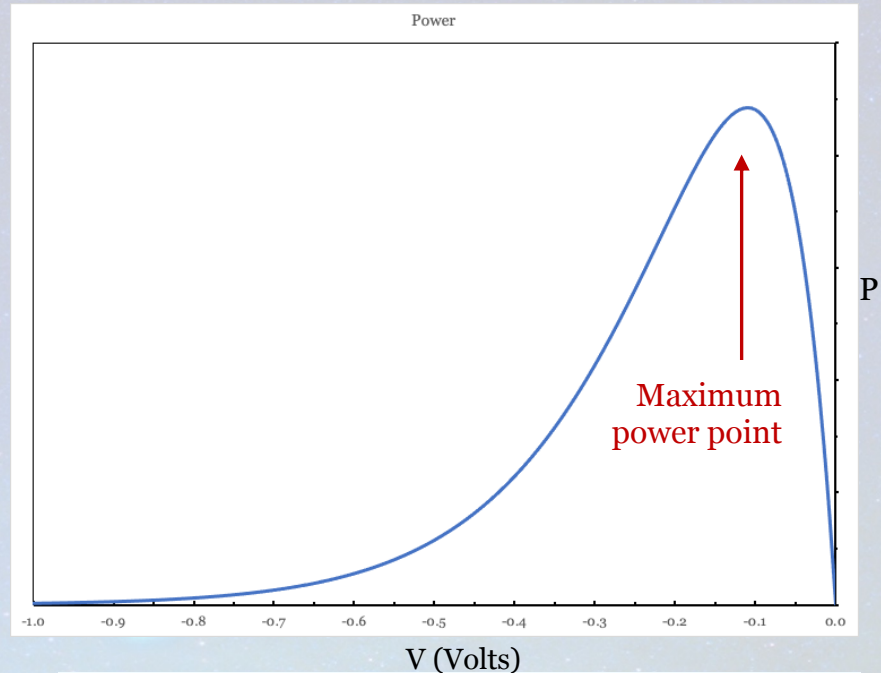
for the simplified calculation, we assume that $T_{external} << T_{cell}$, so the external environment can be ignored

- Power is current times voltage

- Current goes as $I_o e^{-(E_b+V)/kT}$ (*)

  – This is the thermal distribution of carriers (Boltzmann distribution)

  – E_b is barrier voltage

  – Current drops exponentially as you move to high (negative) bias on the IV curve

- Voltage is applied (bias) voltage

  ➢ Power $\sim V I_o e^{-(E_b+V)/kT}$

Power

V (Volts)

Maximum power point

P

Output power as a function of bias voltage for idealized thermoradiative diode at 1000° C
(background temperature assumed negligible)

*For solar cells, we usually subtract 1 from this because current =0 at zero bias. In the detailed balance calculation, the -1 term accounts for the external temperature >0.. For T(cell)>>T(external), the -1 is only important far from the maximum power point
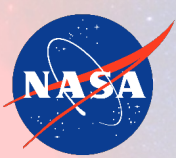
Simplified calculation of Max power point

for the simplified calculation, we assume that $T_{external} \ll T_{cell}$, so the external environment can be ignored

Power $\sim VI_o e^{-(E_b+V)/kT}$

Solve for maximum power

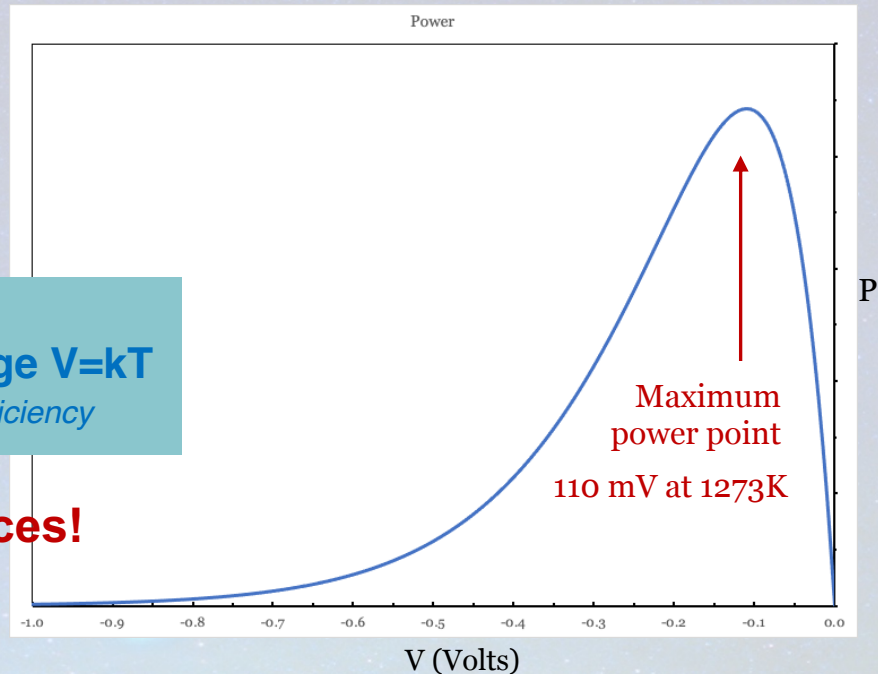- $\frac{d}{dV} VI_o e^{-(E_b+V)/kT} = 0$

Analytical solution:

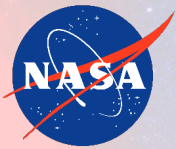**maximum power is at bias voltage V=kT**

– *Note that maximum power point is **not** maximum efficiency*

These are low voltage devices!

25 mV for room temperature (20° C)
100 mV for 900° C

Maximum power point

110 mV at 1273K
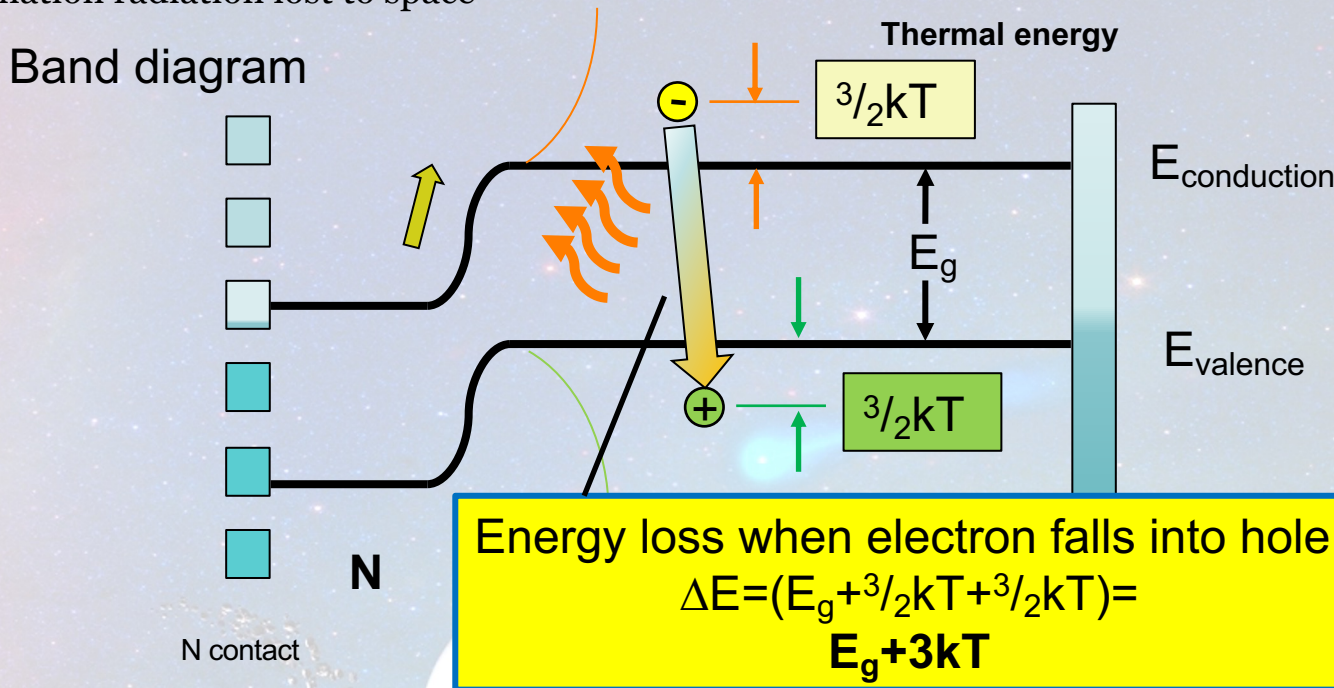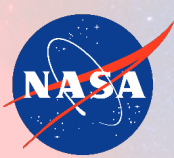
Output power as a function of bias voltage for idealized thermoradiative diode at 1000° C
(background temperature assumed negligible)

- Efficiency = Power produced / (Power Produced + Power Lost)
- In the ideal case (detailed balance, or "Shockley Queisser limit"), the only power loss is the energy of recombination radiation lost to space

Band diagram

Thermal energy

$\frac{3}{2}kT$

$E_{conduction}$

E_g

$E_{valence}$

$\frac{3}{2}kT$

E_e $-$ electrons

E_h $+$ holes

N

N contact

Energy loss when electron falls into hole:
$\Delta E = (E_g + \frac{3}{2}kT + \frac{3}{2}kT) =$
$E_g + 3kT$

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Idealized calculation of highest possible efficiency at Maximum power point

- ➤ Power is current times voltage
- ➤ Power produced is equal to I times bias voltage
- ➤ Voltage lost is equal to I times bandgap plus 3kT/q
  - $-E_g/q$ is bandgap voltage
- ➤ Efficiency = power produced divided by total power
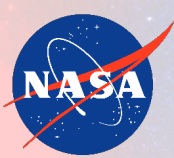 - ➤ $\eta = IV_b / I(V_b+E_g+3kT) = V_b/(V_b+E_g+3kT)$

Power

V (Volts)
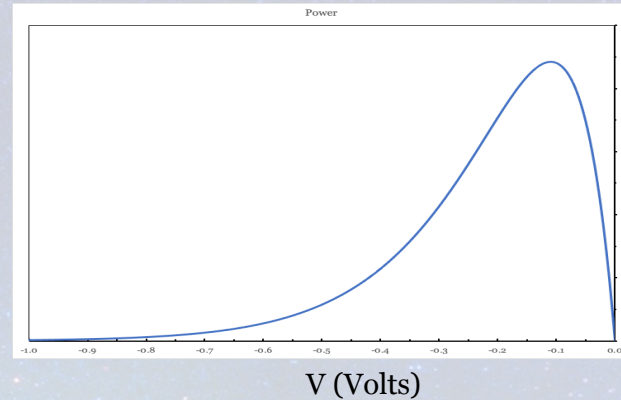
Output power as a function of bias voltage for ideal thermoradiative diode at 1000° C

At maximum power point, bias voltage $V_b = kT$

$$\eta = (kT)/(kT+E_g+3kT)$$

But bandgap must be ≥ 0, so highest efficiency (at maximum power bias) is

➤ $\eta \leq V_b/(V_b+3kt) = 1/4$

Idealized calculation of highest possible efficiency at Maximum power point

Efficiency at max power point is **≤25%**
- Many assumptions in this approximation

At maximum power point, bias voltage $V_b = kT$

$$\eta = (kT)/(kT + \ldots$$

But bandgap must be ≥ 0, so highest eff

➤ $\eta \leq V_b/(V_b+3kt) = 1/4$

Higher than today's thermoelectric converters…
But can't compare real devices with a theoretical limit
- Real world devices never reach ideal efficiency

- The ideal efficiency can be higher than this if the diode is operated at a (negative) voltage greater than the maximum-power voltage

- However, power decreases exponentially as the diode goes to high negative voltages
- Due to non-ideal losses, real-world operating point will tend to be *less* than the ideal maximum-power voltage, rather than higher
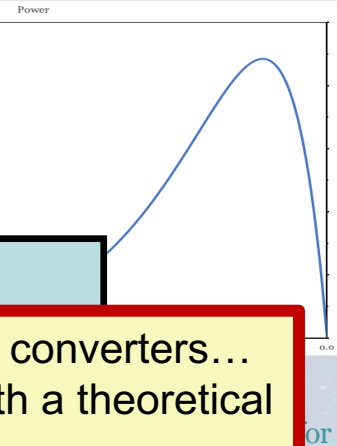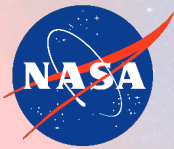
non-ideal losses:
Parasitic thermal emissivity

- All thermal emissivity from the cell other than band to band recombination is parasitic emissivity

- Parasitic emissivity that is radiated into space represents a power loss
  - At constant temperature, this reduces efficiency but does not reduce power output
  - For a constant thermal energy input, increasing radiation will reduce the temperature, and hence decrease the power

- Parasitic emissivity that is not radiated into space, but is absorbed by the diode at energy above the bandgap energy, generates thermophotovoltaic current that subtracts from the thermoradiative current
 - This reduces efficiency *and* power output
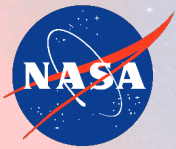
- Parasitic emissivity at energy greater than the bandgap energy generates thermophotovoltaic current that subtracts from the thermoradiative current
- This *reduces the power output* and shifts the maximum-power point to lower voltage
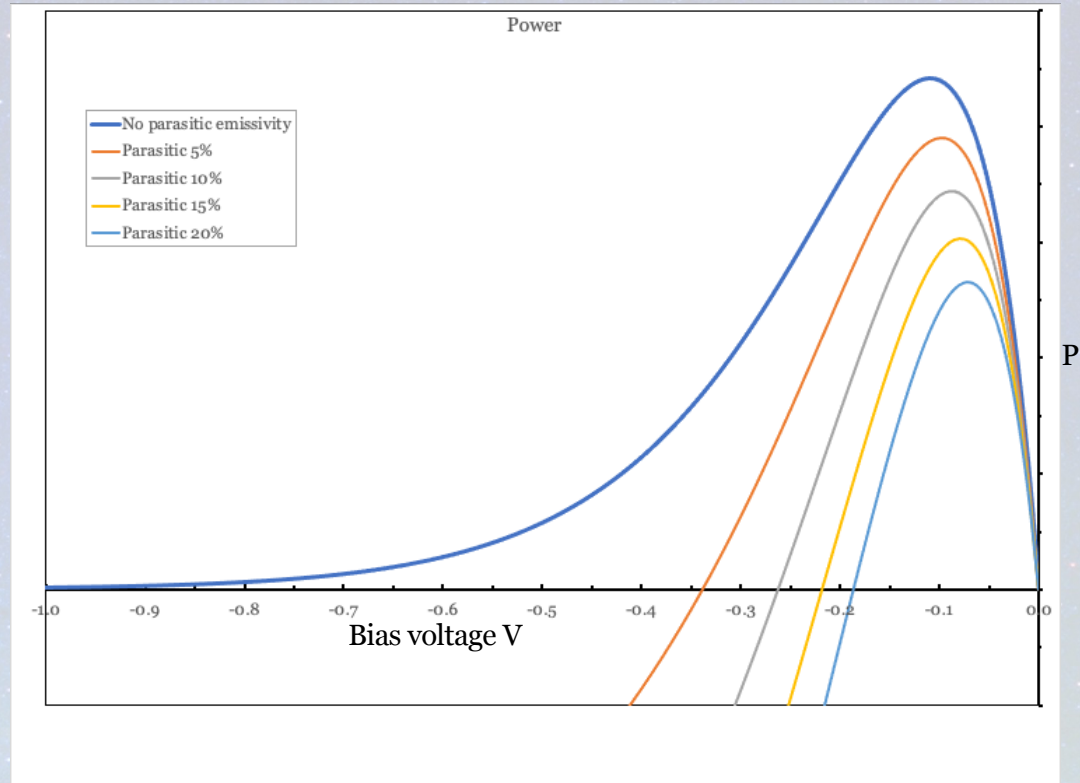
Sources of Parasitic Thermal emissivity: front and back surface

- A thermoradiative array will have a substrate (including back contact metallization) and front surface encapsulation
- These front and back surfaces will be at the cell temperature
- Radiation from these surfaces escaping into space represents an efficiency loss
- Radiation from these surfaces absorbed by the active area will represent a power loss
  - (*for wavelengths shorter than the bandgap cutoff)
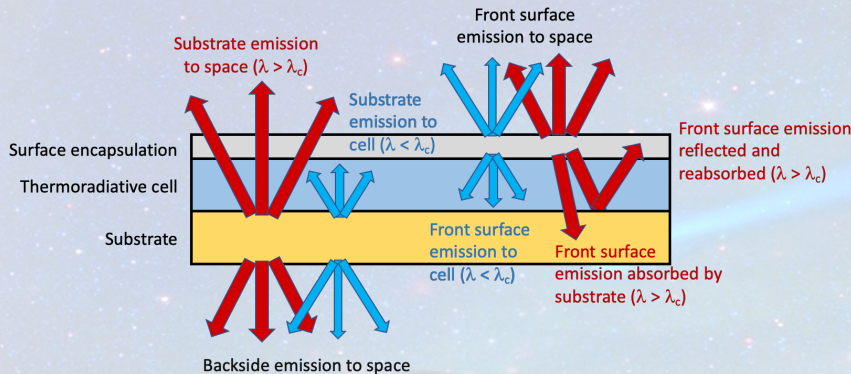
There will also be some parasitic emissivity from the cell itself, which I have left out of this slide for simplicity

Sources of parasitic thermal emissivity: *front and back surface*
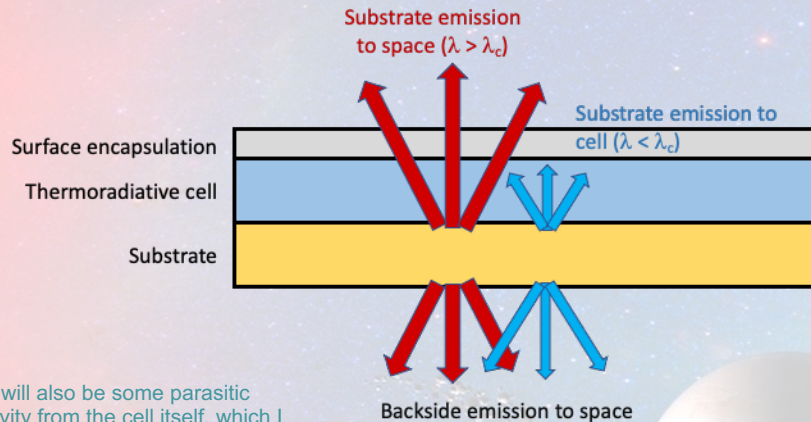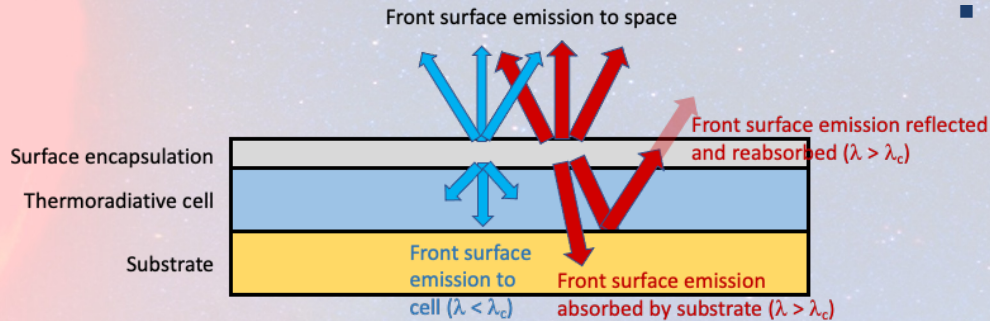
Front surface emission to space

Front surface emission reflected and reabsorbed ($\lambda > \lambda_c$)

Front surface emission to cell ($\lambda < \lambda_c$)

Front surface emission absorbed by substrate ($\lambda > \lambda_c$)

Surface encapsulation

Thermoradiative cell

Substrate
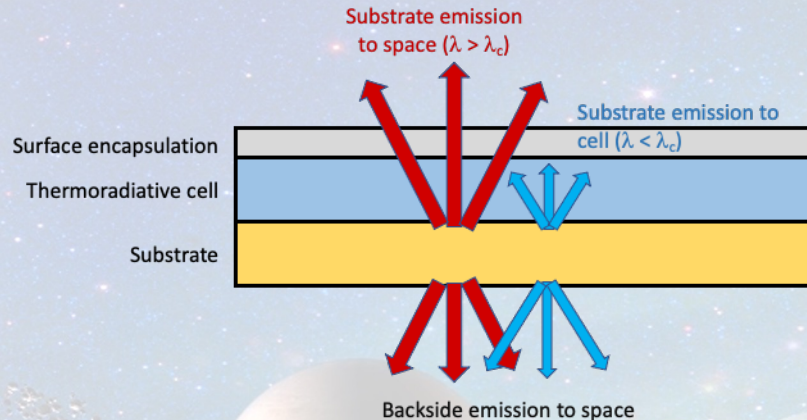
Substrate emission to space ($\lambda > \lambda_c$)

Substrate emission to cell ($\lambda < \lambda_c$)

Surface encapsulation

Thermoradiative cell

Substrate

Backside emission to space

There will also be some parasitic emissivity from the cell itself, which I have left out of this slide for simplicity

- Front surface emission includes thermal emission from encapsulant layers, front metallization, window layers, plus any optical layers (selective reflectors/emitters) on the surface
  - If encapsulant is not perfectly transparent in the IR, it will have some thermal emission
  - The rear substrate is assumed to be non-transmissive to the infrared, so emission from the front is either absorbed or reflected
- Rear surface emission includes thermal emission from the rear metallization, the physical substrate, and any back surface reflectors or insulation layers
  - To minimize heat loss on the rear side, the substrate may be a low emissivity surface, or have insulation added to prevent it from losing heat).
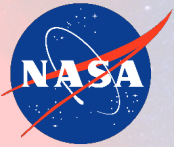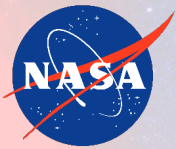
Parasitic thermal emissivity:
front and back surface

- The diode must have contact metallization. Although metals typically have low emissivity, the emissivity is not zero
  - As noted, emissivity back into the cell wavelengths less than λc will subtract from the power.
- Thus, use of a back surface reflector* with high reflectivity near the cut-off wavelength is critical
- For example, a back-surface reflector of 90% reflectivity near the band edge would be adequate for a solar cell, but 10% emissivity could result in thermophotovoltaic carrier generation that could significantly reduce the power. Reflectivity of the back-surface reflector at thermal infrared wavelengths must be very high.

Substrate emission to space ($\lambda > \lambda_c$)

Substrate emission to cell ($\lambda < \lambda_c$)

Surface encapsulation

Thermoradiative cell

Substrate

Backside emission to space

* Kirchhoff's Law of emissivity states that at any given wavelength, reflectivity equals emissivity

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non-ideal losses:
Parasitic Thermal conductivity

- A thermoradiative array will be mechanically mounted. Any support will have some thermal conductivity, which is a thermal conduction path which will leak heat

- A thermoradiative array will require wires to conduct power to the user. The power conductors represent another heat-loss pathway.
  - All heat loss by conduction will be real-world loss of efficiency

Comparison with other solid-state electrical generation

Other forms of solid-state heat engines are thermoelectric and thermophotovoltaic converters.

➢ Each takes heat energy in to produce electrical power with no moving parts.

➢ Each has advantages in different applications

For thermoelectric and thermophotovoltaic conversion, the waste heat radiator is on the **cold** side of the system.

➢ High radiator temperature **decreases** efficiency

For thermoradiative cells, the radiator is the **hot** side of the system

➢ High radiator temperature does not decrease efficiency

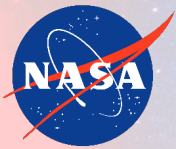# Where are the most valuable applications for thermoradiative cells?

Power Systems in which radiator area is at a premium

- Since thermoradiative cells operate best at high temperature, radiators run hotter, and hence smaller radiators can be used.

Power Systems in which the heat source is low temperature

- Since the cold side of a thermoradiative system is the temperature of deep space (~10K), thermoradiative cells are efficient even at low temperatures*, since the Carnot efficiency loss ($\Delta\eta=T_c/T_h$) is small even at room temperature

*note that although efficiency stays high the actual amount of power produced will be small at low temperatures, since the radiated power is proportional to T^4
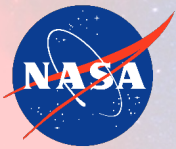
Research problems to be addressed

Demonstrating real-world devices

➢ So far, proof-of-concept devices have been fabricated by a number of groups, which demonstrates that the theory works, but only on very small area diodes, and high efficiency has yet to be demonstrated. We need to prove these devices can achieve high efficiency in the real world!

Real World Losses: Parasitic emissivity

○ The ideal calculation of conversion efficiency assumes *all* of the thermal emissivity is due to band-to-band radiative recombination. This is unrealistic: there will be other emissivity. **The other sources of emissivity are the dominant factor in the losses of the cell.** We need to understand sources of parasitic emissivity and learn to minimize them.

○ In particular, parasitic emissivity at photon energy greater than the bandgap can be re-absorbed by the diode, subtracting from the dark current.

Research problems to be addressed

Manufacturing large-area low-bandgap cells

o We have not yet demonstrated high conversion efficiency on thermoradiative cells. Existing work on low-bandgap materials is in very small area devices, with little or no research on large area devices.

Operating low-bandgap materials at high temperature

o We need to learn how to operate low-bandgap devices at high temperatures. To date little or no work has been done on developing materials characteristics and ohmic contacts for high-temperature operation.

Encapsulation

o Like solar cells, thermoradiative devices must be protected from the space environment. Since glass is opaque to light in the thermal infrared spectrum, new encapsulation techniques will be required.
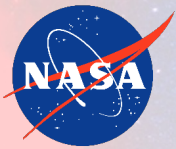
Conclusions

- Thermoradiative cells represent a new type of semiconductor device for converting heat into electrical power

- A simplified analysis was presented, showing the performance near the maximum power point.

- A number of loss mechanisms were identified that lower efficiency below the theoretical maximum. Most critical of these is the effect of parasitic emissivity.

- Much work needs to be done in developing the low-bandgap semiconductors and the technology needed to put these into arrays.

Acknowledgement