Designing a 350nm Ultraviolet Light Emitter with GaN Nanocrystal

Chase A. Lotito, *SIUC Undergraduate*

Abstract—**Using an online simulator, we wish to make a** $350nm$ **ultraviolet light emitting device out of** GaN **nanocrystal. By changing the height of the box nanocrystal, we will quantumly constrain the electrons and cause their bandgap energy to change to the energy needed for a 350nm-wavelength photon.**

I. INTRODUCTION

From Einstein, we know photons of discrete frequencies are emitted from de-energizing electrons. If we could harness these emitted photons, maybe we could get wavelength-specific light sources that are more efficient than their incandescent counterparts.

Ultraviolet light-sources have uses in sanitation, medical, and law enforcement. Manufacturing with a material like GaN will be a large step forward to improving our qualities of life. With efficient use of resources, these nanocrystal devices can find uses in developing nations who can be provided cheaper nanoscale electronic devices.

So, we need to find a way to engineer the specific wavelength of light we need. Our goal is to manipulate the quantum confinement on the electrons in a GaN box-shaped nanocrystal.

Ultraviolet radiation's wavelength falls in between $400nm$ and $1nm$. To get the design frequency $f_d = 350nm$, we would need higher frequency ultraviolet light from our GaN nanocrystal. We can find the exact frequency for light in free-space:

$$f = \frac{c}{\lambda} \qquad (1)$$

$$\implies f_d = \frac{3 \times 10^8}{350 \times 10^{-9}} = 8.571 \times 10^{14} Hz$$

From here, we can use the Planck-Einstein relation, to find the necessary bandgap energy E_g.

$$E_g = hf \qquad (2)$$

$$\implies E_g = (6.626 \times 10^{-34})(8.571 \times 10^{14}) = 3.545eV$$

Here, E_g really represents the difference in energy from the first-excited energy state E_1 and the ground energy state E_0, $h = 6.626 \times 10^{-34} \ J \cdot s$, and f is the frequency of the particle.

Now, it is not certain that nature allows for a continuous frequency GaN electrons. For a given crystal, we know from Schrodinger's wave equation Ψ that the energy states for its electrons has been discretized by the potential boundaries it imposes. So, if we can change the potentials we can tailor E_g to our desired frequency.

Ultimately, we achieve this by manipulating the volume of a cube GaN nanocrystal by changing it's height L_z. The different heights might constrain or relieve the wavefunction of the electrons giving rise to different bandgaps.

II. DESIGN METHOD

From nanoHUB, the *Nanoscale Solid-State Lighting Device Simulator* [1] from Southern Illinois University Carbondale, we can simulate GaN nanocrystals of different shapes, calculating the 3-D wavefunctions for the device.

We will sweep the height of the nanocrystal L_z from 1nm-6nm, and use Microsoft EXCEL to find a polynomial regression $E_g(L_z)$ that approximates the bandgap energy E_g with respect to L_z.

The resulting function for bandgap will let us predict the value for L_z for $E_g = 3.545eV$. It will also be valuable to see how dE_g/dL_z will show intuition on quantum constraining.

III. DISCUSSION ON DESIGN AND ANALYSIS

From our sweep across values of L_z, we were able to get the following polynomial approximation for E_g with respect to L_z ($R^2 = 0.9946$):

$$E_g(L_z) = 0.0002L_z^6 - 0.0077L_z^5 + 0.112L_z^4$$
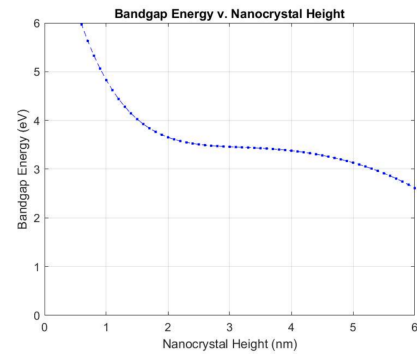$$- 0.8339L_z^3 + 3.3261L_z^2 - 6.7689L_z + 9 \quad (3)$$

Fig. 1. E_g versus L_z

Using MATLAB, we can find when $L_z = 2.3nm$, $E_g(2.3) = 3.545eV$.

Now, the simulator only calculates the wavefunction for integer multiples of $0.5nm$, so we cannot verify our value for L_z, but a close approximation is fine.

We can also use MATLAB to graph the derivative of Eq. 3.

What we find is large changes in the bandgap energy for values of L_z between $0nm - 2nm$.

This is the region that the quantum confinement is stronger than the natural confinement that a bulk piece of GaN provides to an electron.

We would need a better approximation for Eq. 3, but we can predict that as $L_z \to \infty$, we would find $E_g \to E_{g0}$, where E_{g0} is the *bulk bandgap energy* of GaN .
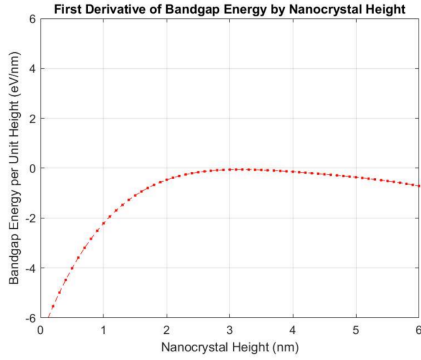

Fig. 2. $dE_g \ dL_z$

A. Why does the bandgap vary with L_z?

Remember for the wavefunction solved for a electron in an infinite potential well, the wavenumber k_n was:

$$k_n = \frac{n\pi}{L} \tag{4}$$

This equation showing that the wavenumber is inversely proportional to the dimensions of the quantum confinement. And, in the k-space, energyis inversely proportional to that dimension squared.

$$E \propto 1/L^2 \tag{5}$$

This proportionality follows with what we have in Fig. 1. Differences in the actual bandgap energy function we simulated comes from the specific crystal lattice with crystal potential U_c.

Speaking in terms of the Heisenberg Uncertainty principle, the narrower the confinement of our electrons, the more certain their position can be in all of space, and this causes a larger spread for the electron's momentum. As $\Delta p \propto \Delta E$, we get more energy for more localized particles. Then, by providing different dimensional constraints on the electron, we can engineer the correct bandgap energy for 350nm light.

IV. CONCLUSION

REFERENCES

[1] S. S. Ahmed, "Nanoscale solid-state lighting device simulator," https://nanohub.org/resources/nanossl, 2019.