A MONTE-CARLO MODEL OF RESONANT RADIATION TRANSPORT IN A PLASMA DISPLAY PANEL: TRANSITION FROM OPTICALLY THICK TO OPTICALLY THIN REGIMES

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Plasma Display Panels (PDPs) - How They Work

- A dielectric barrier discharge is initiated in a mixture of inert gases, usually He and/or Ne with a small admixture of Xe.

- UV radiation produced by resonant transitions of Xe and non-resonant relaxation of Xe$_2^*$ is converted to visible light using phosphors.

- Schematic of PDP cell. Voltage is applied to the top electrode. The bottom electrode is grounded. Barrier ribs are opaque to UV radiation.

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Temporal Evolution of Xe \((5p^56s)\) Density

- **He/Ne/Xe = 70/26/4, 400Torr**
- Snapshot of Xe density \((m^{-3})\) at various times during the voltage pulse applied to the upper electrode while the lower electrode is held at ground potential.
Radiation Trapping

- Xe (5p$^6$6s - 5s$^2$5p$^6$, 147nm) and (5p$^6$6s$'$ - 5s$^2$5p$^6$, 129nm) resonant photons are in a quasi-optically thick regime

\[ \lambda_{o,\text{abs}} \ll d \text{ typical cell dimensions} \]

- Photons are re-absorbed and re-emitted many times before leaving the discharge

- Each time a photon is re-absorbed it can be ‘lost’ via collisional quenching of the excited atomic state

\[
\begin{align*}
\text{Xe} + h\nu & \xrightarrow{\text{resonant re-absorption}} \text{Xe}^* \\
\text{Xe}^* & \xrightarrow{\text{resonant radiation}} \text{Xe} + h\nu \quad \text{photon still available}
\end{align*}
\]

or

\[
\begin{align*}
\text{Xe}^* + M_1 & \xrightarrow{\text{collisional quenching}} \text{Xe} + M_2 \quad \text{photon lost}
\end{align*}
\]
Resonant vs Excimer UV Radiation

$R_Q << (\tau_{\text{rad}})^{-1}$  Collisional quenching rates are 2-3 orders of magnitude smaller than the radiative decay rate.\[ \Rightarrow \] Radiative decay is the dominant de-excitation process for Xe*

$\lambda_{o,\text{abs}} / d \sim 10^3$  Resonant photons re-absorbed & re-emitted many times \[ \Rightarrow \] Residence time in discharge is greatly increased \[ \Rightarrow \] Quenching rates increase - photon loss increases

Radiation from the non-resonant relaxation of Xe$_2^*$ is *not* trapped
Flux to phosphor depends only on the geometry of the PDP cell

*In order to optimize the luminous efficiency of the PDP cell an accurate picture of radiation transport is required.*
Resonant Radiation - Thick or Thin?

- Radiation trapping has previously been accounted for by using Holstein factors to describe the apparent lengthening of the lifetime of the resonant states (Holstein [1]).

- To use Holstein factors to determine the fraction of resonant radiation leaving the discharge, an assumption must be made about the opacity of the radiation throughout the line shape and at all positions in the discharge.

- The combination of gas pressures and PDP cell dimensions is such that the resonant radiation may be optically thick near line center and optically thin in the wings of the emission line shape - i.e., in a partially optically thick regime.
Limitations of the Holstein Factor Approach

- Radiation transport models that use the Holstein factor can give very different results depending on the assumptions made about the opacity of the resonant radiation.

- **Optically thin**: all photons eventually leave the discharge, resonant radiation dominates the UV flux to the phosphor [2],[3]

- **Optically thick**: only photons emitted near edge of discharge escape, excimer radiation dominates the UV flux to the phosphor [4]
Previous Radiation Transport Models

Summary of existing PDP models that include a treatment of resonant radiation trapping based on the Holstein factor ($\tau_{\text{rad,eff}} = \tau_{\text{rad}} \times H$)

  Assumed optically thin conditions - power radiated per unit surface area is given by integrating the product (density of radiating species x decay rate) over the electrode gap
  Key result - light output is dominated by resonant radiation.

  Assumed optically thin conditions - UV emission ~ average UV photon density between electrodes
  key result - < 10% Xe  UV emission is dominated by resonant radiation.
  > 20% Xe  UV emission is dominated by excimer radiation.

  Assumed optically thick conditions - only resonant radiation emitted within a few absorption lengths of the phosphor reaches it.
  key result - UV flux to the phosphor is dominated by excimer radiation.
Partial Frequency Redistribution

Most photons are emitted with $\nu \sim \nu_o$ where $g(\nu)$ is greatest for resonant absorption.

There is a small probability that the photon will be emitted from the wings of the line shape where the cross-section for resonant re-absorption is low.

These photons have a higher probability of eventually escaping the discharge.

However,

\[ \lambda_{\text{abs}} \sim \frac{1}{g(\nu)} \]

Most photons are emitted with $\nu \sim \nu_o$ where $g(\nu)$ is greatest.

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OPTICAL AND DISCHARGE PHYSICS
Monte-Carlo Frequency Redistribution Model

The Monte-Carlo Frequency Redistribution (MC-FR) model is an off-line radiation transport module of a self-consistent PDP discharge simulation developed at the University of Illinois (Rauf and Kushner [4]).

The MC-FR model is invoked periodically during the PDP simulation to calculate resonant UV transport throughout the discharge.

- *Primary* photon - a single quanta of energy transferred to a Xe atom by an inelastic collision, subsequently emitted as a photon

- Distribution of *primary* photons in 2\(d\) in proportion to the density of radiating species

- Pressure and Doppler broadening are both important.
  Initial photon frequencies are randomly chosen from the Voight line shape function using the method of *joint and conditional probability density functions* (Lee [5]).
Sampling the Voight Profile

- Voight line shape
  \[ g(\bar{V}) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-y^2}}{a^2 + (\bar{V} - y)^2} dy \]

- Frequency departure from line center in units of Doppler width
  \[ \bar{V} = (v - v_0) / \Delta v_D \]

- Doppler width
  \[ \Delta v_D = \sqrt{\frac{8k_BT}{Mc^2v_0}} \]

- Homogeneous linewidth
  \[ \Delta v_H = \frac{1}{2\pi} [(A_{21} + k_1 + k_2 + 2v_{col})] \]

- Radiative lifetimes, \(A_{21}\)
  \[ \text{Xe}(5p^56s) \quad A_{21} = 2.9 \times 10^8 \text{s}^{-1} \]
  \[ \text{Xe}(5p^56s') \quad A_{21} = 4.05 \times 10^8 \text{s}^{-1} \]

- Quenching rates \(k_1, k_2\)
  Obtained from look-up tables as a function of \(T_e\) or \(E/N\) calculated by solving Boltzmann’s Equation (Rauf and Kushner [4]).

- Elastic collision frequency for Xe with heavy particles calculated using the first Lennard-Jones parameter and the thermal speed of the Xe atoms
  \[ v_{col} = \sum_j \pi (\sigma_{LJ})^2 v_{th}^j N_j \]
Monte-Carlo Frequency Redistribution Algorithm.

- Photon frequencies are randomly selected from a Voight lineshape

- Two step sampling:
  1) Randomly select Xe velocity $v$ from a normal distribution
  2) Substitute $v$ into Lorentzian lineshape

initialize next photon

$x = x + \delta x$

photon hit surface?

record properties

invoke boundary conditions

photon exited mesh?

traversed $\lambda_{abs}$?

null absorption

photon absorbed?

select new $\nu$
calculate $\lambda_{abs}$

photon re-emitted?
Conditions for this Study

- Gas mixture: Ne/He/Xe = (30-\(x\))/70/\(x\) \(x = 0.001 - 25\)
- Pressure: 400 Torr
- Cell dimensions: 210\(\mu\)m x 210\(\mu\)m
- Dielectric separation: 150\(\mu\)m
- Barrier ribs (width): 15\(\mu\)m
- Magnitude of voltage pulse \(V_0\), applied to upper electrode was adjusted to give an average peak electron density of \(\sim 1\times10^{18} \text{ m}^{-3}\).

For the range of Xe concentrations studies here \(V_0 = 210-500\text{V}\)
Escape Probability vs Xe Concentration

Escape Probability - the fraction of primary photons that escape from the discharge

- Escape probabilities as a function of Xe concentration for primary UV photons emitted by the resonant transitions:
  - Xe \((5p^56s \rightarrow 5s^25p^6)\)
  - Xe \((5p^56s' \rightarrow 5s^25p^6)\)

- Escape probabilities have been calculated for photons that:
  1. leave the discharge, and
  2. reach the phosphor

- As the fraction of Xe in the gas mixture is increased, radiation is trapped in the discharge for longer times
  - other quenching processes can compete with radiative emission
  - lower escape probabilities

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Transport Regimes

- **Optically thin**
  - Low (<0.1%)
  - Too few Xe atoms to cause appreciable trapping

- **Partially thick**
  - Medium (1-10%)
  - Trapping increases. Quenching, which is dominated by other Xe atoms, becomes significant. Escape probability begins to fall.
  - *PDP cells are typically operated in this regime.*

- **Optically thick**
  - High (>10%)
  - $\lambda_{\text{abs}}$ very short. Collisional quenching competes with radiative decay. < 5% primary photons escape.
Partial Frequency Redistribution

Spectra of Xe (5p\textsuperscript{5}6s - 5s\textsuperscript{2}5p\textsuperscript{6}) Photons Incident on the Phosphor for Varying Xe Concentration.

**Low Xe Concentration**
- radiation is not heavily trapped
- spectrum of radiation leaving the discharge is essentially the Voight line shape, with a small depletion near line center

**Higher Xe concentration**
- \( \lambda_{\text{abs}} \) decreases - significant trapping and quenching.
- Observed emission spectrum becomes progressively depleted near line center and accentuated in the wings.
Effect of Quenching on Escape Probability

- Temporal evolution during a single voltage pulse of
  (a) escape probabilities
  (b) volume averaged electron densities
  for varying Xe mole fractions.

- Before the discharge ignites the escape probability is at a maximum.

- \( n_e \) and \( T_e \) increase during the current pulse, increasing the electron impact quenching rates

- Escape probability decreases markedly.

- After the discharge is extinguished however, the escape probabilities return to their initial values.
Non-Local Resonant Radiation Transport

• The density of sites from which primary photons incident on the phosphor were last emitted - an effective source function for untrapped primary photons.

• **Optically thick** radiation - source function peaks adjacent to the phosphor.

• **Optically thin** radiation - more extended source functions.

• Separating the source functions into 3 frequency bands illustrates the role of frequency redistribution in the non-local nature of resonant photon transport.
0.1% Xe Concentration

- 65% photons reaching phosphor are emitted further than 40µm (~100 $\lambda_{abs,o}$) away

- Photons with $\nu \sim \nu_o$ are more likely to be emitted near the phosphor

- Photons emitted from the wings are more likely to originate in the center of the PDP cell where the Xe* density is greatest

LINE CENTER

(a) $|\nu-\nu_o|/\Delta\nu_D| < 3$
MAX = $2.57 \times 10^{-3}$

(b) $3 < |\nu-\nu_o|/\Delta\nu_D| < 10$
MAX = $1.10 \times 10^{-3}$

(c) $|\nu-\nu_o|/\Delta\nu_D| > 10$
MAX = $5.05 \times 10^{-4}$
1% Xe Concentration

- 65% photons reaching phosphor are emitted further than 20µm (~500 $\lambda_{\text{abs,0}}$) away

As Xe concentration is increased $\lambda_{\text{abs}}$ decreases, increasing the chance of photon loss via quenching.

However, frequency redistribution is more effective, increasing the fraction of photons that reach the phosphor from distances further than 50µm.

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4% Xe Concentration

- 71% photons reaching the phosphor are emitted further than $10 \mu m \sim 1000 \lambda_{o,abs}$ away.

- 20% are emitted further than $50 \mu m \sim 5000 \lambda_{o,abs}$ away.

(a) $|(v - v_o)/\Delta v_D| < 3$

MAX = $2.57 \times 10^{-3}$

(b) $3 < |(v - v_o)/\Delta v_D| < 10$

MAX = $1.10 \times 10^{-3}$

(c) $|(v - v_o)/\Delta v_D| > 10$

MAX = $5.05 \times 10^{-4}$

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Fraction of Xe($5p^56s - 5s^25p^6$) photons incident on the phosphor that were emitted further than distance $d$ ($\mu$m) from phosphor, for varying concentrations of Xe.

- At low Xe concentration the source of resonant UV flux to the phosphor is distributed throughout the volume of the discharge.
- As the fraction of Xe in the gas mixture is increased the transition from optically thin to optically thick radiation transport is apparent.
Contribution from Wings of the Lineshape

Relative contributions of $\text{Xe}(5p^56s - 5s^25p^6)$ photons incident on the phosphor from the three frequency bands

- At low Xe concentrations most of the resonant radiation reaching the phosphor is emitted from the core of the line shape.

- As the Xe concentration is increased radiation trapping & frequency redistribution become stronger - emission is increasingly from the wings of the line shape.
Key Results

- At low Xe concentration (0.001-0.1%) radiation trapping and quenching are not important. Almost 100% of the resonant UV photons eventually escape the discharge. Roughly 30% reach the phosphor.

- As the Xe concentration is increased to values at which PDP cells are typically operated (1-10%), escape probabilities begin to fall rapidly. $\lambda_{\text{abs}}$ scales inversely with Xe concentration, increasing the degree of photon trapping and quenching. The contribution of Xe resonant radiation to the production of visible light is ultimately limited.

- Assumptions of optically thin or optically thick radiation are not appropriate for PDP operating conditions. A significant fraction (~30% at 4% Xe concentration) of the resonant UV flux to the phosphor is emitted further than 35 $\mu$m away. More than 50% of these photons were emitted with frequencies further than 10 Doppler widths from the center of the emission line shape.
References


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