Soot Light Absorption and Its Optical Band Gap

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Motivation

Soot particles contribute to global warming by their strong light absorption. However, assessments of the impact of soot on climate change are hindered by the large uncertainty of their optical properties. Soot optical band gap can be used to accurately quantify the evolving refractive index of soot and correlate it to soot maturity [1]. Here, the optical band gap of soot is measured for two premixed flames with different equivalence ratios. It is shown that volatile organic carbon (VOC) significantly changes the soot light absorption and optical bandgap. Once VOC is removed, the measured band gap of the large soot particles compares well with values reported for mature soot [2]. For small particles, the measured bandgap correlates well with the values suggested by the quantum confinement theory, indicating that soot optical bandgap monotonically decreases with increasing mobility size [3].

Band Gap of Incipient, Nascent and Mature Soot

Optical Band Gap (eV) as sampled
washed once
washed twice
HAB = 5.5 mm
Φ = 2.40

Mean Mobility Diameter, \( \langle d_m \rangle \) (nm)

6.7 9.5 13.1 14.5

Optical Band Gap (eV)

5.5 10.0

Soot optical band gap decreases monotonically from 1.4 to 0.2 eV, by increasing soot mobility diameter and maturity as particles grow in the flame.

Obtaining Soot Band Gap from Absorbivity

Tauc relation

<table>
<thead>
<tr>
<th>Linearization</th>
<th>Region I</th>
<th>Region II</th>
<th>Region III</th>
<th>Max ( R^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>0.84</td>
<td>1.01</td>
<td>2.66</td>
<td>4.66</td>
</tr>
</tbody>
</table>

Soot band gaps are obtained using the Tauc relation based on the multiwavelength absorbivity curves. Observing linear regions with different slopes suggests mixing of particles with different bad gaps [8].

References


Funding

1. Soot optical band gap decreases with increasing soot maturity and size.
2. Volatile Organic Carbon condensed on the surface of soot pamps could significantly change their light absorption properties.

Conclusions

The measured soot optical band gaps agree well with the values calculated with the quantum confinement theory [3] suggesting that particle size and maturity evolve together in the flamer.