Diffractive Imaging of Coherent Nuclear Motion in I_2

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Observing the motion of the nuclear wave packets during a molecular reaction, in both space and time, is crucial for understanding and controlling the outcome of photoinduced chemical reactions. In this work we use wave packet simulation to imaged the motion of a vibrational wave packet in isolated iodine molecules using ultrafast electron diffraction

The standard methods of gas electron diffraction (GED) is used to extract the molecular structure from the diffraction patterns. Under the independent atom approximation, for randomly oriented molecules, the total scattering intensity I_{tot} can be written as the sum of the atomic scattering intensity I_{at} and the molecular scattering intensity I_{mol}

$$I_{at}(s) = \sum_{i=1}^{N} \left| f_i(s) \right|^2$$

$$I_{mol}(s,t) = \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left| f_i(s) \right| \left| f_j(s) \right| \cos(\eta_i - \eta_j)$$

$$\int \frac{\sin(sR)}{sR} P_{ij}(R,t)\, dr$$

The structural information of the molecule is usually extracted through the modified diffraction intensity,

$$sM(s,t) = s \frac{I_{mol}(s,t)}{I_{at}(s)}$$

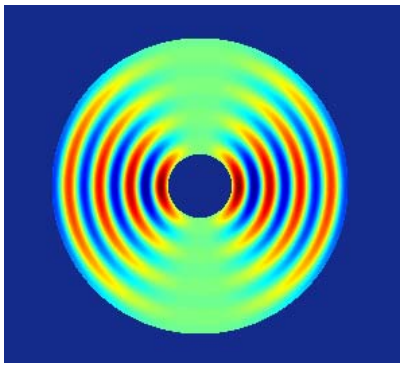

Figure 1. The diffraction pattern of I_2 at the delay time of 217 fs after the 530 nm femtosecond pump laser pulse.

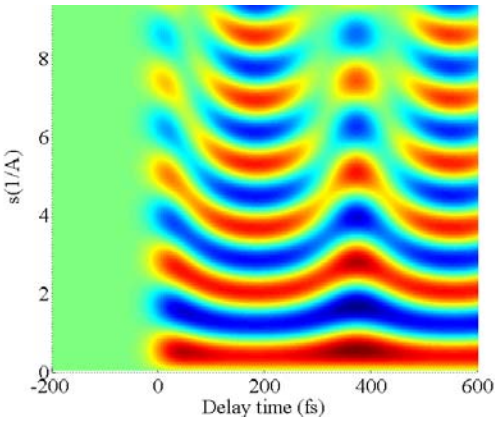

Figure 2. The time-resolved modified scattering intensity difference of I_2 after excitation by a 530 nm laser pulse

Reference

[1] J. Yang *et al*. 2016 *Phys. Rev. Lett.* **117** 153002

[2] J. Yang *et al*. 2016 *Nat. Commun*. **7** 11232

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