Supplementary Information to accompany:

Spatially Resolved Optical Emission and Modelling Studies of Microwave-Activated Hydrogen Plasmas Operating under Conditions Relevant for Diamond Chemical Vapor Deposition

Edward J.D. Mahoney,[1,2] Benjamin S. Truscott,[1,a] Sohail Mushtaq,[1] Michael N.R. Ashfold,[1] and Yuri A. Mankelevich [3]

[1] School of Chemistry, University of Bristol, Bristol, U.K. BS8 1TS

[2] Centre for Doctoral Training in Diamond Science and Technology, University of Warwick, Gibbet Hill Road, Coventry, U.K., CV4 7AL

[3] Skobel'tsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie gory, Moscow, 119991 Russia

[a] Present address: Element Six Global Innovation Centre, Harwell Campus, Fermi Ave, Didcot, U.K., OX11 0QR

Figure S1

(a) $I_{em}(\lambda, z)$ Image (where $z = 0$ defines the substrate surface) in the wavelength range 423-497 nm from a hydrogen plasma operating under base conditions: $p = 150$ Torr, $P = 1.5$ kW, $F(H_2)$ = 300 sccm, $d_{sub} = 32$ mm and $d_{wire} = 0.01$". The strong lines at 434.0 nm and 486.1 nm are the H Balmer-γ and Balmer-β emissions. (b) $I_{em}(\lambda)$ plot of the summed emission intensities in the height range $3 \leq z \leq 6$ mm over the wavelength range $448 \leq \lambda \leq 465$ nm, with R branch lines of the G-B (0,0) band identified.
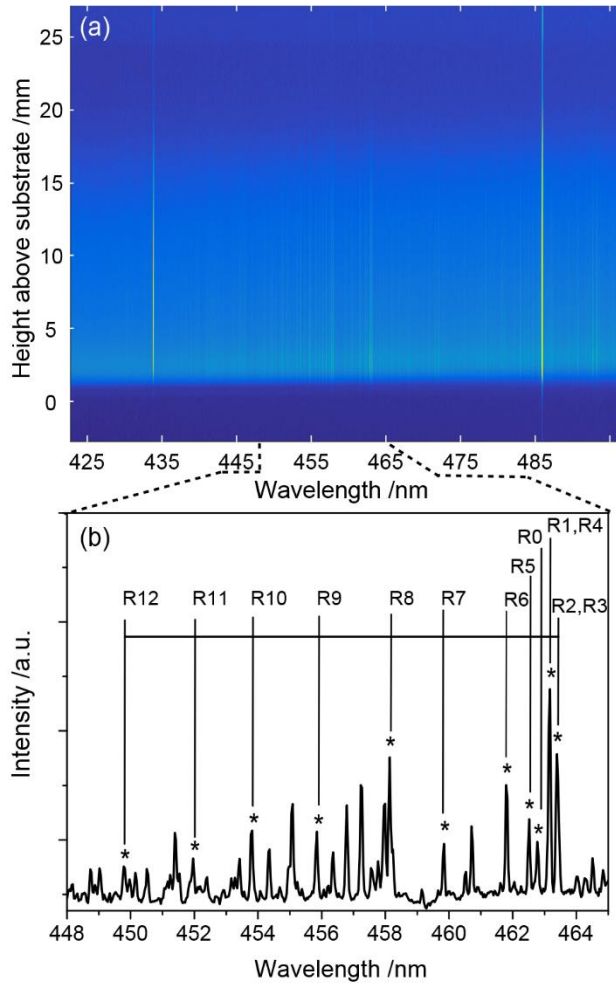
Figure S2

(a) $I_{em}(\lambda, z)$ image (where $z = 0$ defines the substrate surface) in the wavelength range 563-636 nm from a hydrogen plasma operating under base conditions: $p = 150$ Torr, $P = 1.5$ kW, $F(H_2)$ = 300 sccm, $d_{sub} = 32$ mm and $d_{wire} = 0.01"$. (b) $I_{em}(\lambda)$ plot of the summed emission intensities in the height range $3 \leq z \leq 6$ mm over the range $600 \leq \lambda \leq 620$ nm, with the utilised H_2 d-a (0,0) Q branch lines identified.
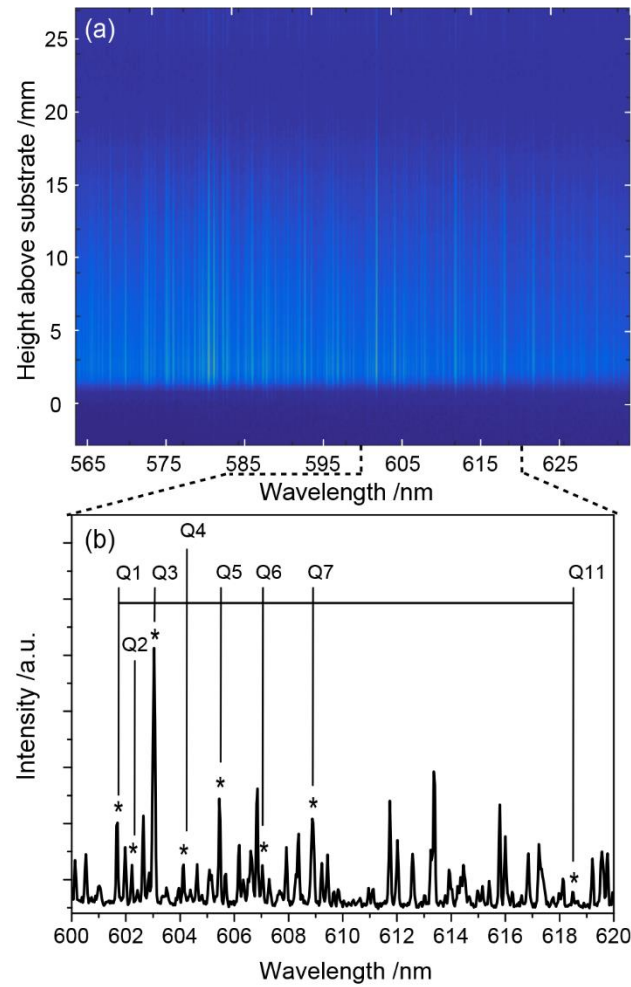
Figure S3

Spatial profiles of (a) $I_{em}(H_2^*,$ d–a) emission and (b) $I_{em}(H_\alpha)$ emission for a MW activated hydrogen plasma operating at three pressures with a substrate diameter $d_{sub} = 17$ mm, $d_{wire} = 0.004"$ and $P = 0.9$ kW. The relative intensities in any given plot are displayed on a common vertical scale. Tilt view images of the plasma above the substrate (indicated by the ellipse superposed on the $p = 275$ Torr image), aperture by the slot shaped viewing port, are shown in the inset in (b). The T_{sub} values at all three pressures were below our detection limit.
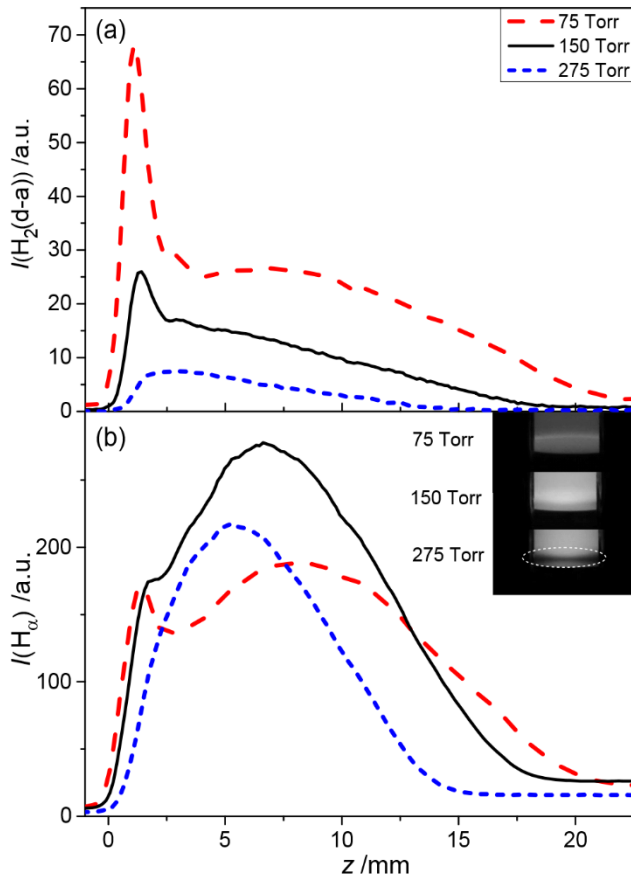
Figure S4

Spatial profiles of (a) $I_{em}(H_2*,$ d–a) emission and (b) $I_{em}(H_\alpha)$ emission from a MW activated hydrogen plasma operating at three pressures with a substrate diameter d_{sub} = 17 mm, d_{wire} = 0.004", and P = 1.85 kW. The relative intensities in any given plot are displayed on a common vertical scale. The inset in (b) shows tilt view images of the plasma above the substrate, apertured by the slot shaped viewing port. The measured T_{sub} values are, respectively, below detection limit, 1020 ˚C and 1070 ˚C for p = 75 Torr (red), 150 Torr (black) and 275 Torr (blue).
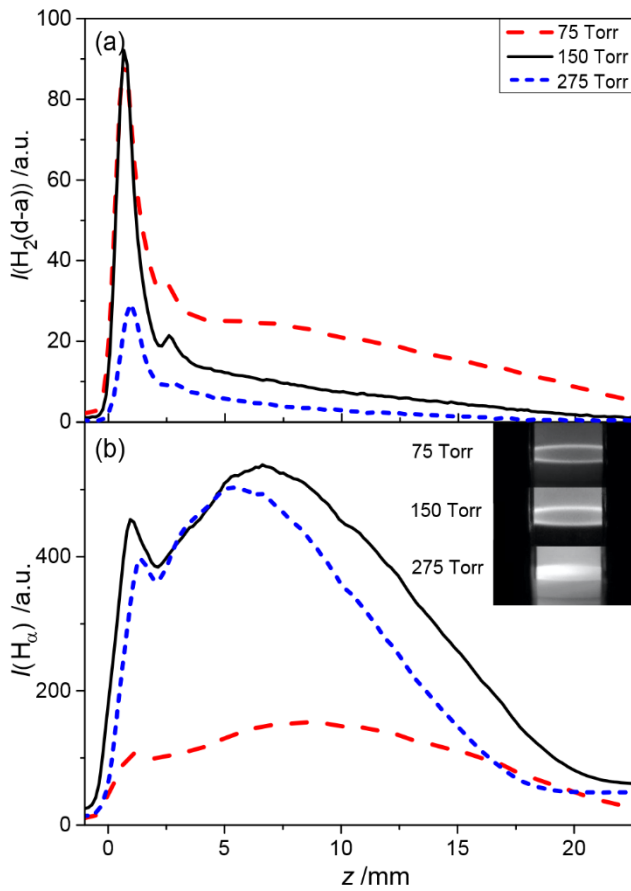
Figure S5

Calculated (a) axial (z, $r = 0$) and (b) radial ($z = 10.5$ mm, r) distributions of T_g, T_e and T_{tail} (left hand axis) and the average absorbed MW power density $|jE|$, and electric $|E|$ and reduced electric $|E|/(N \times a)$ fields (right hand axis) for $d_{sub} = 18$ mm and base conditions of p and P.
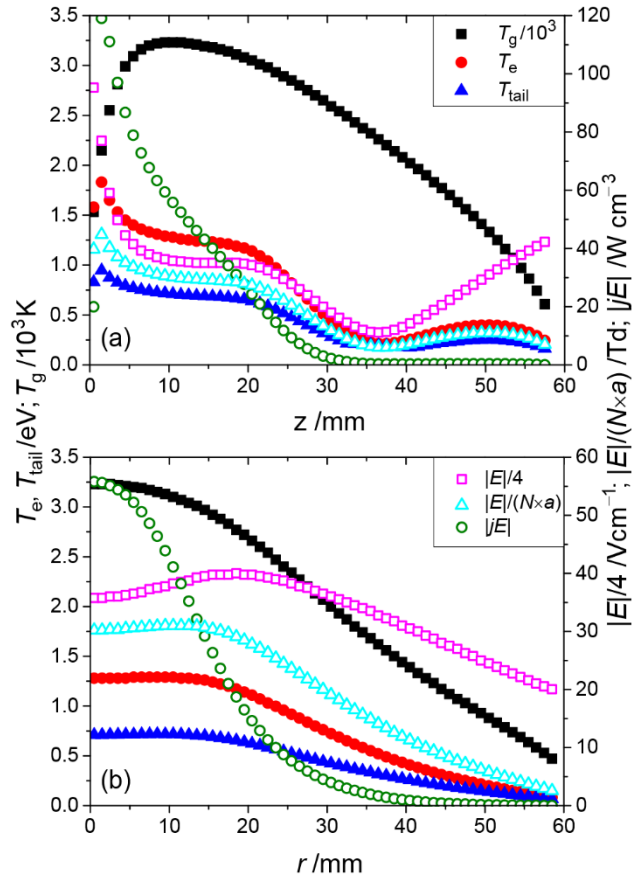
Figure S6

Calculated axial (z, $r = 0$) concentration distributions of (a) H(n = 1, 2, 3) atoms, (b) the dominant charged species and (c) the ground and selected excited states of H_2 for d_{sub} = 18 mm and base conditions of p and P. Note that the distributions in (a) and (c) are plotted on a logarithmic scale.
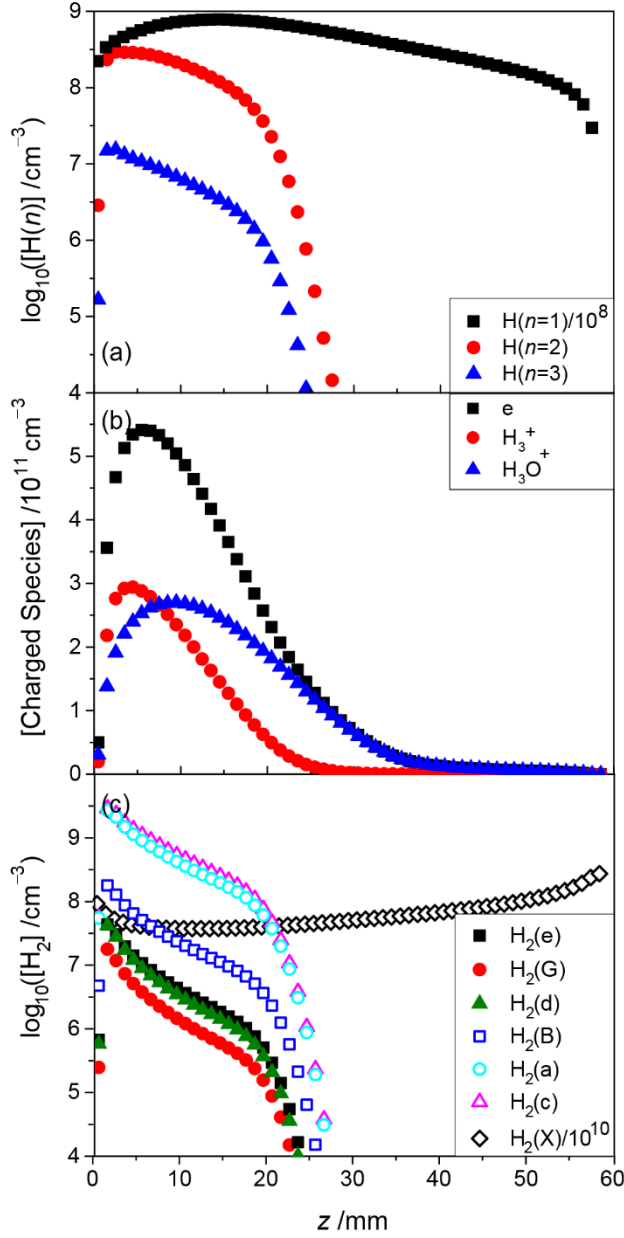
Figure S7

Calculated radial (z = 10.5 mm, r) concentration distributions of (a) H(n = 1, 2, 3) atoms, (b) the dominant charged species and (c) the ground and selected excited states of H_2 for d_{sub} = 18 mm and base conditions of p and P. Note that the distributions in (a) and (c) are plotted on a logarithmic scale.
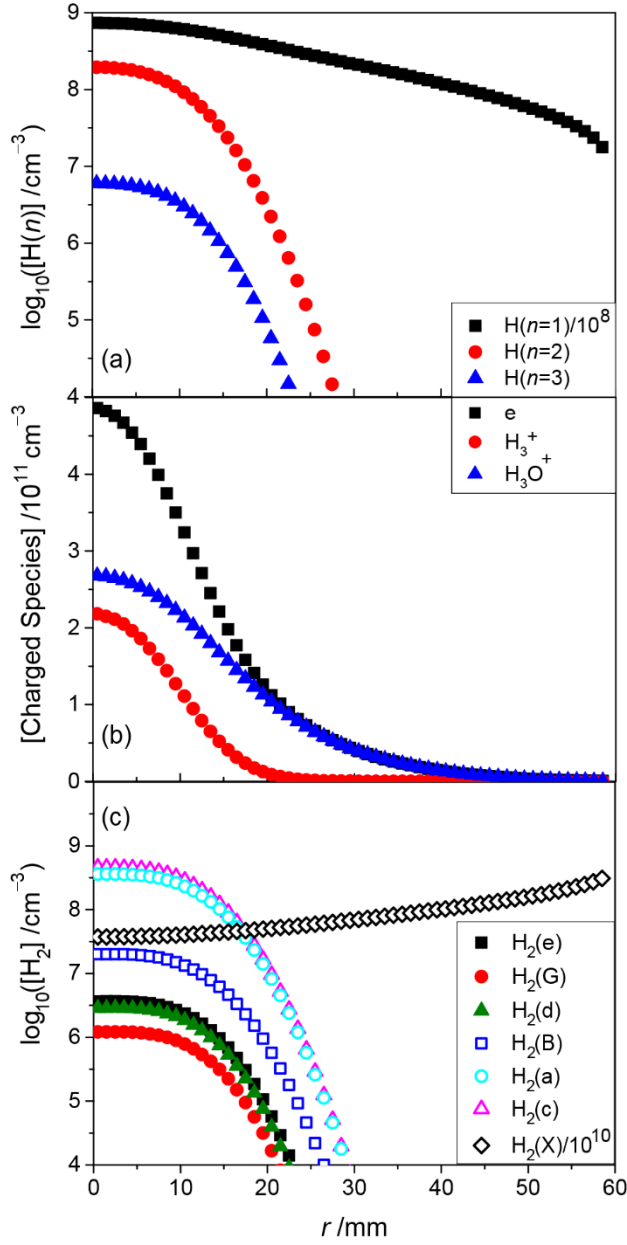
Figure S8

Comparisons of the calculated column densities (symbols) and measured emission intensities (lines) of (a) $H_2(G, v = 0)$ and (b) $H_2(d, v = 0)$ molecules for $p = 75$ Torr (red), 150 Torr (black) and 250 Torr (blue), with $P = 1.5$ kW and $d_{sub} = 32$ mm.
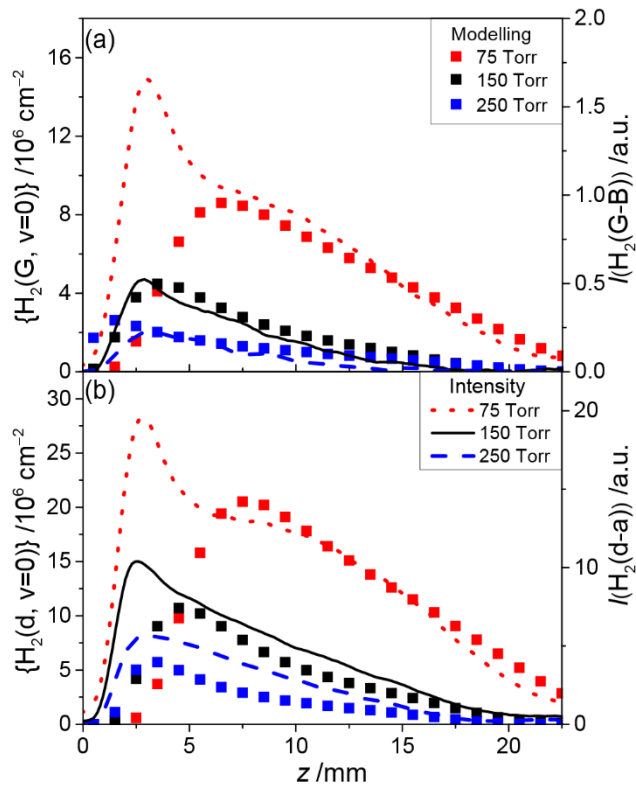
Figure S9

Comparisons of the calculated column densities (symbols) and measured emission intensities (lines) of (a) $H_2(d, v = 0)$ and (b) $H(n = 3)$ atoms for $d_{sub} = 17(18)$ mm (in the experiment (in the modelling), in red) and $d_{sub} = 32$ mm (black), with $P = 1.5$ kW, $p = 150$ Torr and $d_{wire} = 0.01''$.