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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

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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-$\gamma$ and Balmer-$\beta$ 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) $I_{em}(H_α)$ emission from a MW activated hydrogen plasma operating at three pressures with a substrate diameter $d_{sub} = 17$ mm, $d_{wire} = 0.004^\prime\prime$, 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 \((z = 10.5 \text{ mm}, r)\) distributions of \(T_g\), \(T_e\) and \(T_{\text{tail}}\) (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 \(d_{\text{sub}} = 18 \text{ mm}\) 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 $d_{\text{sub}} = 18$ 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 H₂ 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 $d_{\text{sub}} = 32$ mm.
Figure S9

Comparisons of the calculated column densities (symbols) and measured emission intensities (lines) of (a) $\text{H}_2(d, v = 0)$ and (b) $\text{H}(n = 3)$ atoms for $d_{\text{sub}} = 17(18)$ mm (in the experiment (in the modelling), in red) and $d_{\text{sub}} = 32$ mm (black), with $P = 1.5$ kW, $p = 150$ Torr and $d_{\text{wire}} = 0.01”$. 