Supplementary information

Elucidating interfacial parameters of platinum–palladium bulk alloy single crystals

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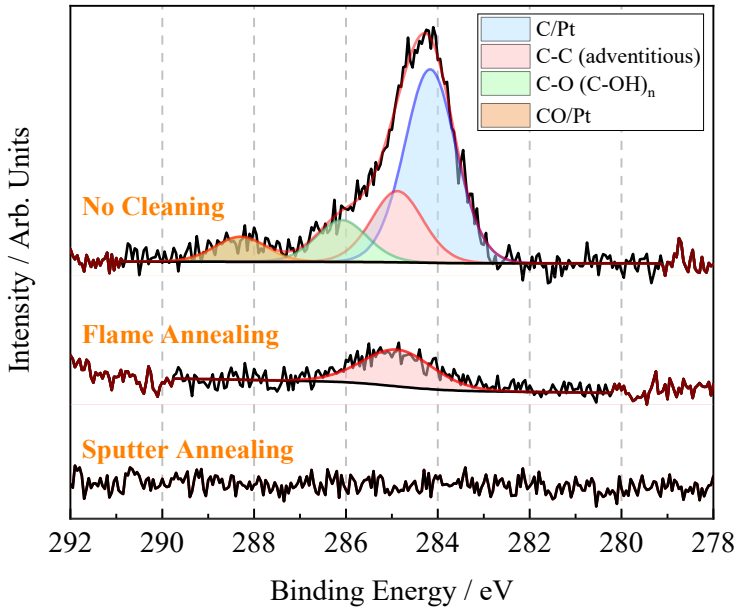


Figure S1. XPS C1s spectra of an as-prepared, flame-annealed, and sputter-annealed Pt(100) single crystal.

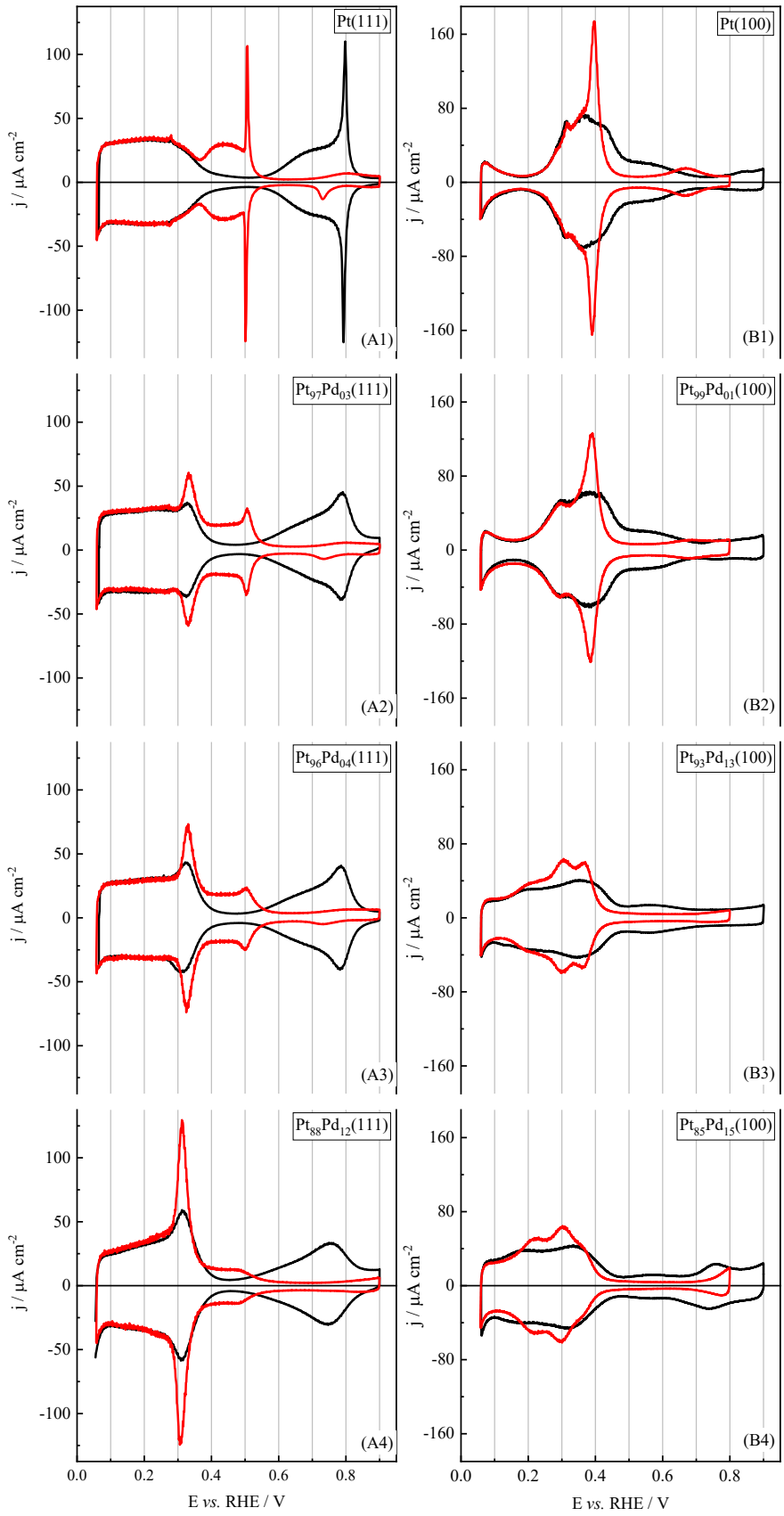


Figure S2. Comparison of the voltammetric profiles of the (A1-A4) $Pt_{100-x}Pd_x(111)$ and (B1-B4) $Pt_{100-x}Pd_x(100)$ surfaces, recorded at 0.05 $V \cdot s^{-1}$, in (black line) 0.1 $mol.L^{-1}$ $HClO_4$ and (red line) 0.1 $mol.L^{-1}$ H_2SO_4.

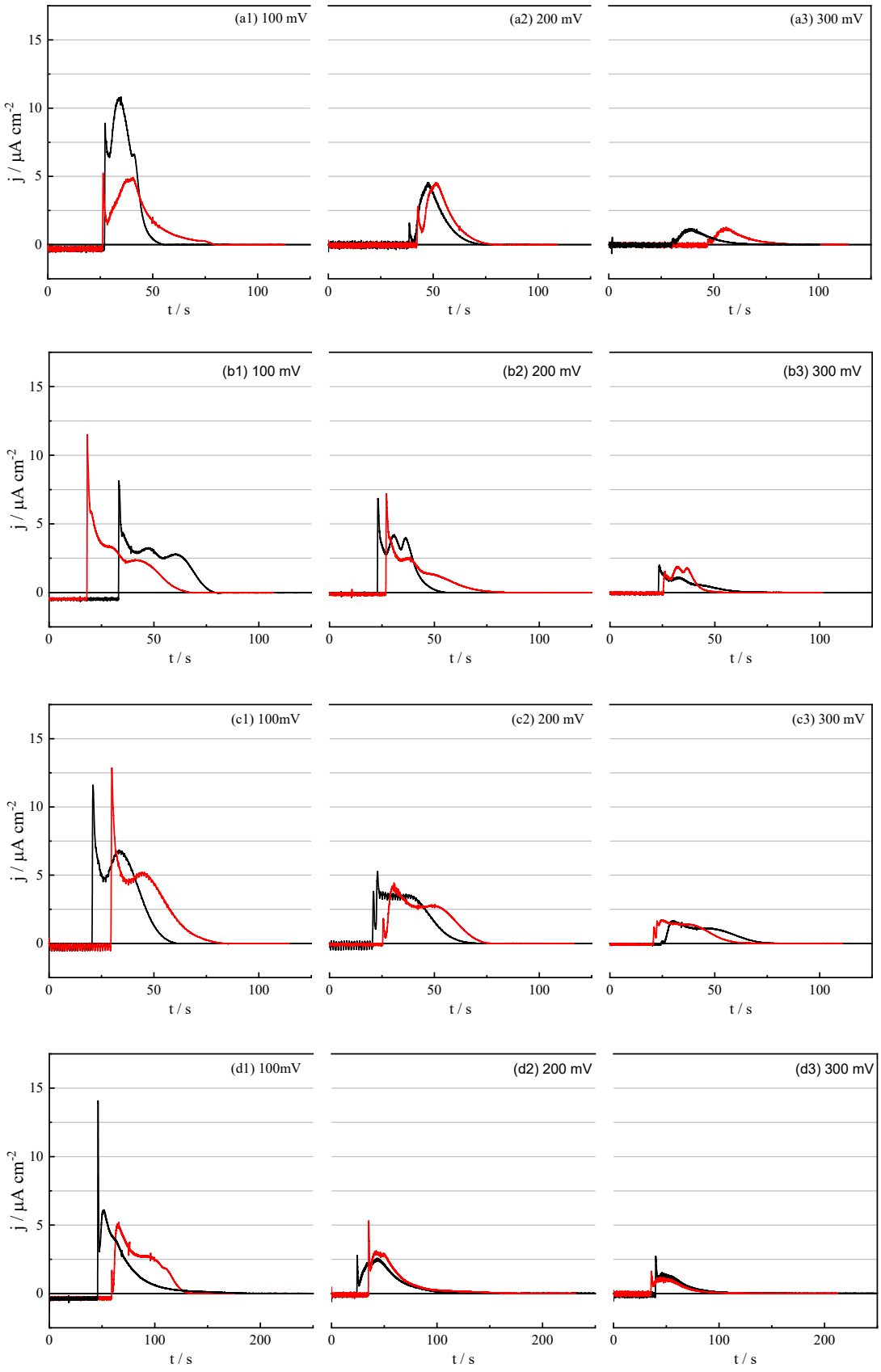
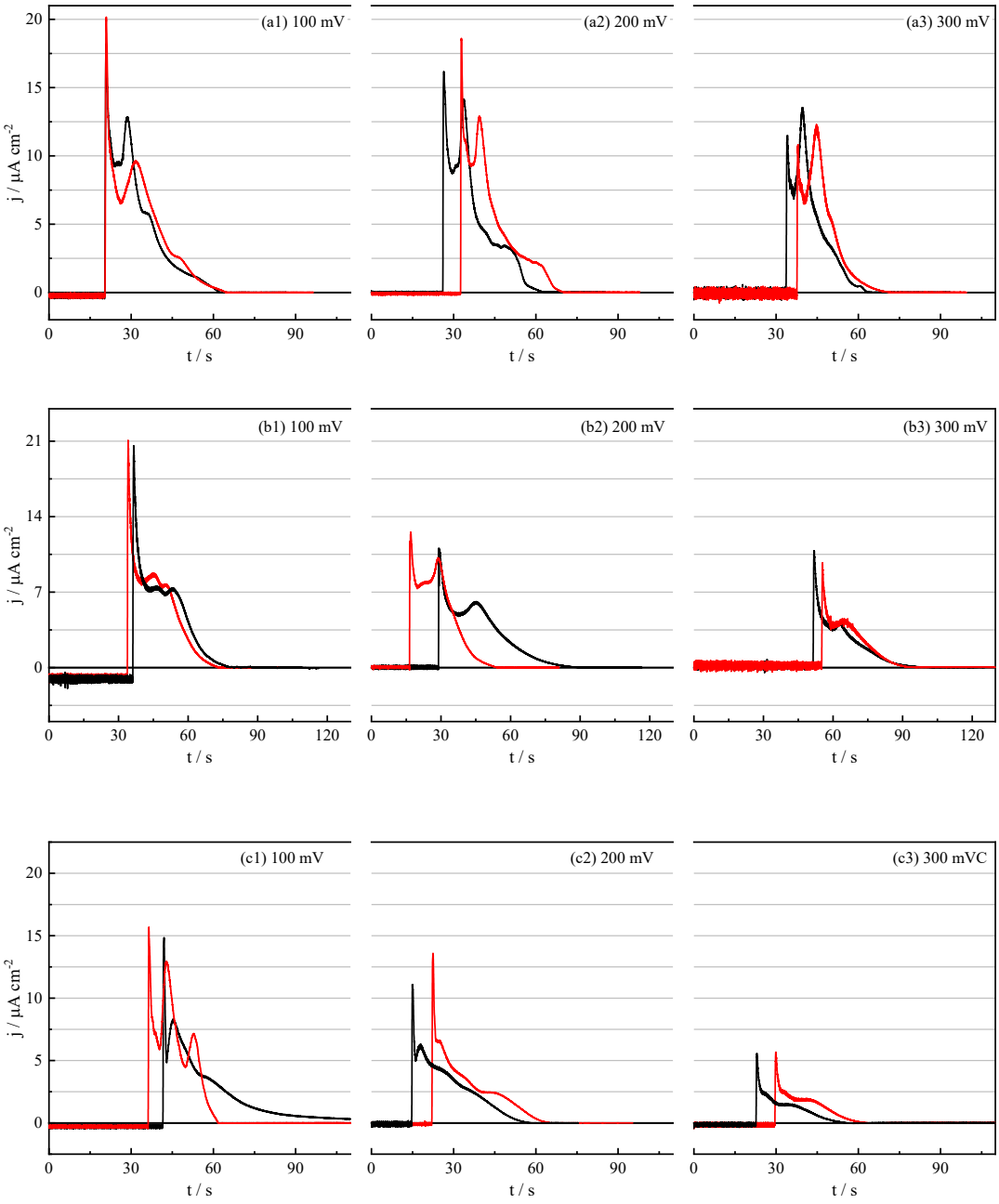

(a1) 100 mV
(a2) 200 mV
(a3) 300 mV
(b1) 100 mV
(b2) 200 mV
(b3) 300 mV
(c1) 100mV
(c2) 200 mV
(c3) 300 mV
(d1) 100mV
(d2) 200 mV
(d3) 300 mV
j / μA cm-2
t / s

Figure S3. Typical transient of current for CO displacement at (a1-d1) 100 mV, (a2-d2) 200 mV, and (a3-d3) 300 mV for (a) Pt(111), (b) $Pt_{97}Pd_{03}$(111), (c) $Pt_{96}Pd_{04}$(111), and (d) $Pt_{88}Pd_{12}$(111) surface in 0.1 mol L^{-1} $HClO_4$. The black and red curves are the results of experiments repeated on different days.

Table S1. Charge density measured during CO displacement experiments at 0.10, 0.20, or 0.30 V on Pt(111) or PtPd(111) family. Numerical value of the charge density with the error is the mean value and the standard deviation, respectively, determined by replicating the experiments 3 or more times.

E *vs.* RHE / V	**Charge / μC cm^{-2}**			
	Pt(111)	$Pt_{97}Pd_{03}$(111)	$Pt_{96}Pd_{04}$(111)	$Pt_{88}Pd_{12}$(111)
0.100	141.5 ± 1.5	137.6 ± 0.4	155.5 ± 0.5	159 ± 3
0.200	62 ± 4	85.5 ± 0.4	102.2 ± 0.9	92 ± 3
0.300	18.0 ± 0.3	29.0 ± 0.7	40.0 ± 0.6	35 ± 3


(a1) 100 mV
(a2) 200 mV
(a3) 300 mV
(b1) 100 mV
(b2) 200 mV
(b3) 300 mV
(c1) 100 mV
(c2) 200 mV
(c3) 300 mVC
j / μA cm-2
t / s

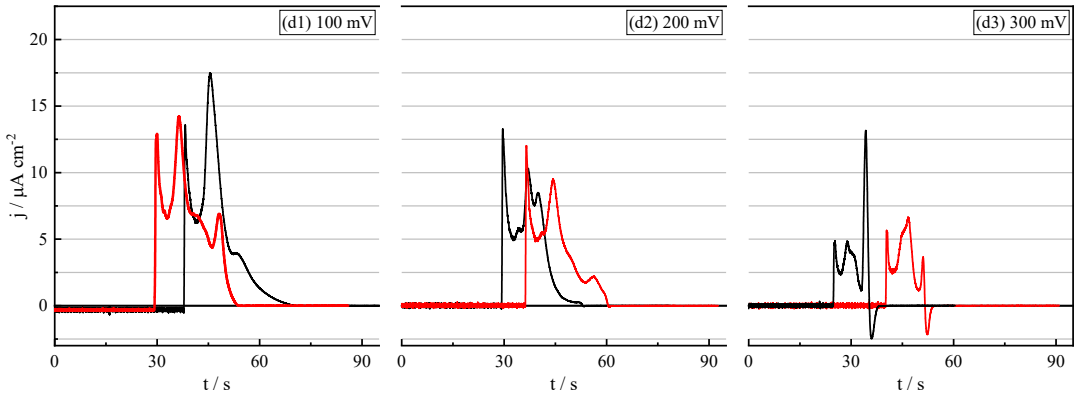


Figure S4. Transient of current for CO displacement at (a1-d1) 100, (a2-d2) 200, and (a3-d3) 300 mV for (a) Pt(100), (b) $Pt_{99}Pd_{01}$(100), (c) $Pt_{93}Pd_{07}$(100), and (d) $Pt_{85}Pd_{15}$(100) surface in 0.1 mol L^{-1} $HClO_4$. The black and red curves are the results of experiments repeated on different days.

Table S2. Charge density measured during the displacement of CO experiments at 0.10, 0.20, or 0.30 V on Pt(100) or PtPd(100) family.

E *vs.* RHE / V	**Charge / µC cm^{-2}**			
	Pt(100)	$Pt_{99}Pd_{01}$(100)	$Pt_{93}Pd_{07}$(100)	$Pt_{85}Pd_{15}$(100)
0.100	202 ± 3	209 ± 3	171 ± 6	176 ± 6
0.200	186 ± 1	177 ± 2	123 ± 4	119 ± 3
0.300	135 ± 4	92 ± 6	47 ± 5	39.0 ± 0.5

Table S3. Supplemental information about CO oxidation on Pt(111) and PtPd(111) family.

SURFACE	Integrated Charge /µC cm^{-2}	Total charge at 0.90 V /µC cm^{-2}	Corrected Charge /µC cm^{-2}	E_{peak} / V
Pt(111)	487 ± 6	166	321 ± 5	0.755 ± 0.005
$Pt_{97}Pd_{03}$(111)	485 ± 10	153	332 ± 10	0.761 ± 0.009
$Pt_{96}Pd_{04}$(111)	501 ± 5	159	342 ±5	0.772 ± 0.005
$Pt_{88}Pd_{12}$(111)	486 ± 5	166	320 ± 5	0.764 ± 0.004

Table S4. Supplemental information about CO oxidation on Pt(100) and PtPd(100) family.

SURFACE	Integrated Charge	Total charge at 0.85 V/µC cm^{-2}	Corrected Charge	E_{peak} / V

	/μC cm^{-2}		/μC cm^{-2}	
Pt(100)	490 ± 5	160	330 ± 5	0.738 ± 0.005
$Pt_{99}Pd_{01}$(100)	512 ± 8	166	346 ± 8	0.729 ± 0.007
$Pt_{93}Pd_{07}$(100)	455 ± 4	137	318 ± 4	0.722 ± 0.005
$Pt_{85}Pd_{15}$(100)	511 ± 11	155	356 ± 11	0.7904 ± 0008