2nd International Symposium on Master Engineering

Booklets

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Author: JUAREZ-ROBLES, Daniel

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ECORFAN-México, S.C.
143 – 50 Itzopan Street
La Florida, Ecatepec Municipality
Mexico State, 55120 Zipcode
Phone: +52 1 55 6159 2296
Skype: ecorfan-mexico.s.c.
E-mail: contacto@ecorfan.org
Facebook: ECORFAN-México S. C.
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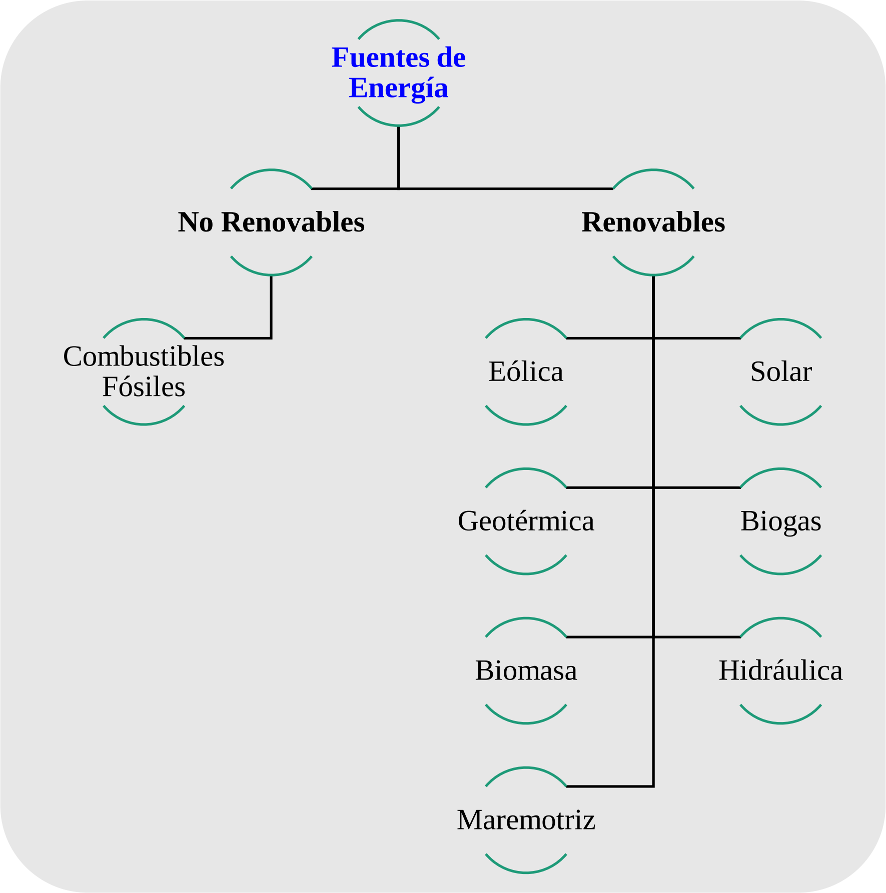
Motivación



Sistemas de Almacenamiento de Energía

- El mundo necesita de la generación conjunta de las diferentes fuentes de energía.
- Los sistemas de almacenamiento de energía almacenan el exceso de energía para luego ser usado en la red eléctrica.

Sistemas de Almacenamiento de Energía

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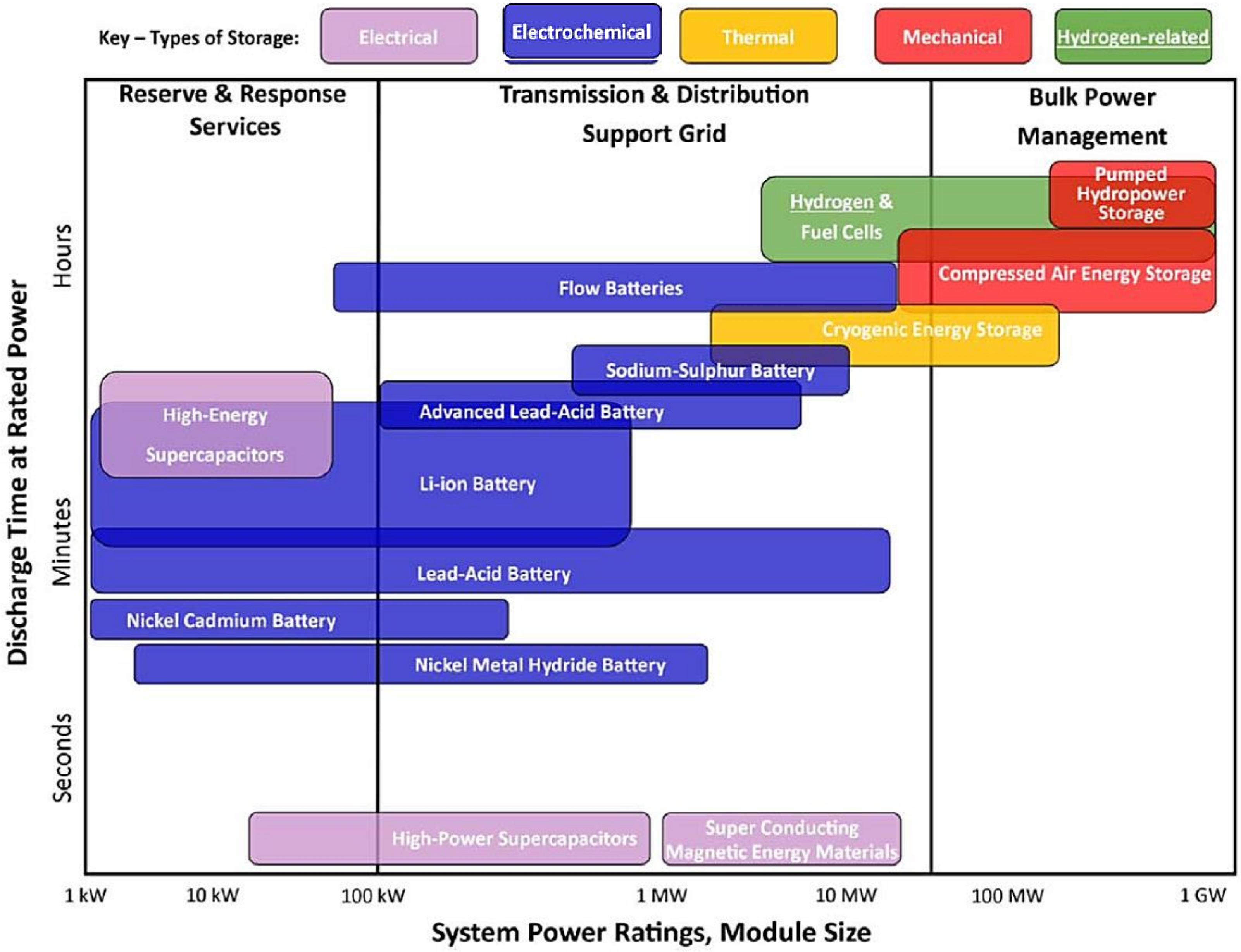


Sistemas Electroquímicos

- Un sistema electroquímico es un dispositivo capaz de **convertir** la **energía química** almacenada en una sustancia **en energía eléctrica** (Descarga).

- La carga de la celda electroquímica se da al usar la energía eléctrica para llevar a cabo una reacción.

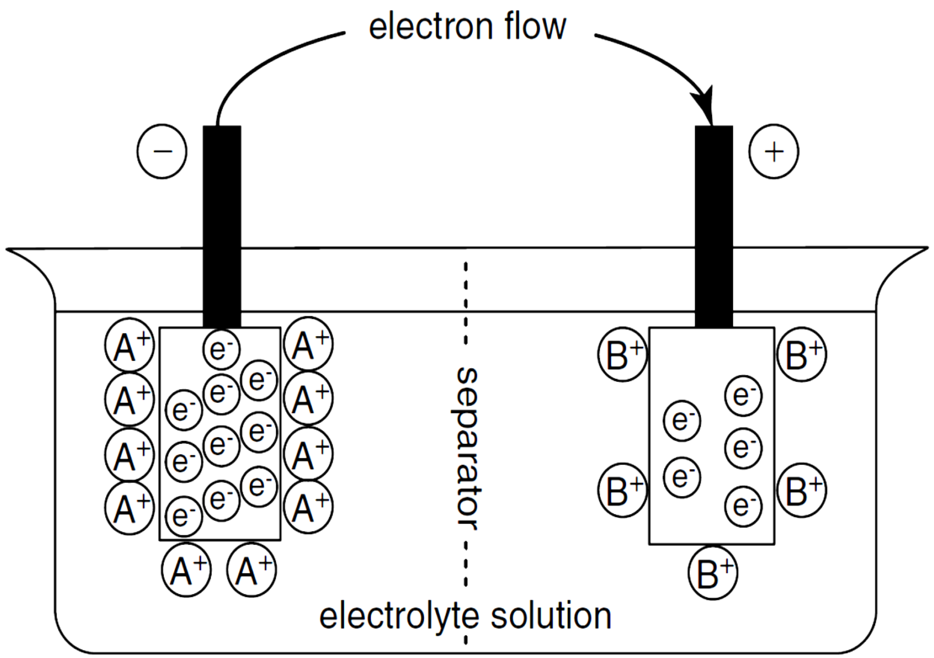


Figure · Celda electroquímica con electrodos positivo y negativo

Reacción Simple

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$

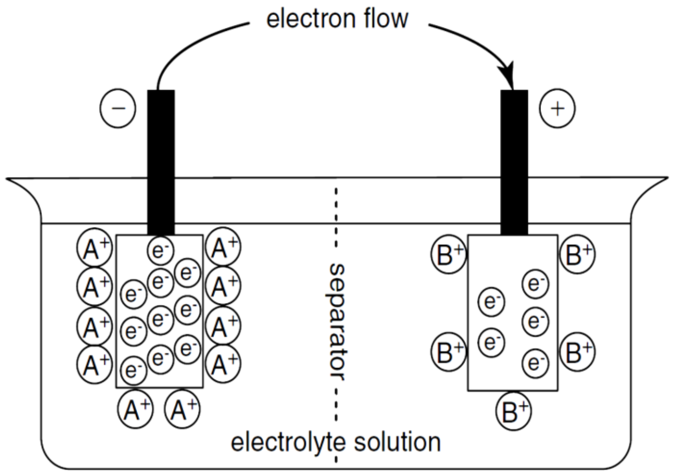
Reacción Electroquímica

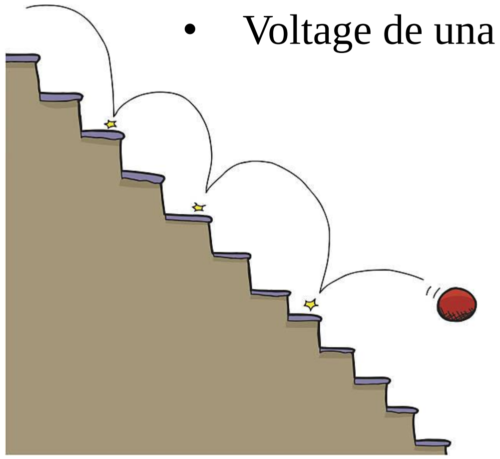
$$H_2 \rightarrow 2H^+ + 2e^-$$

$$\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O$$

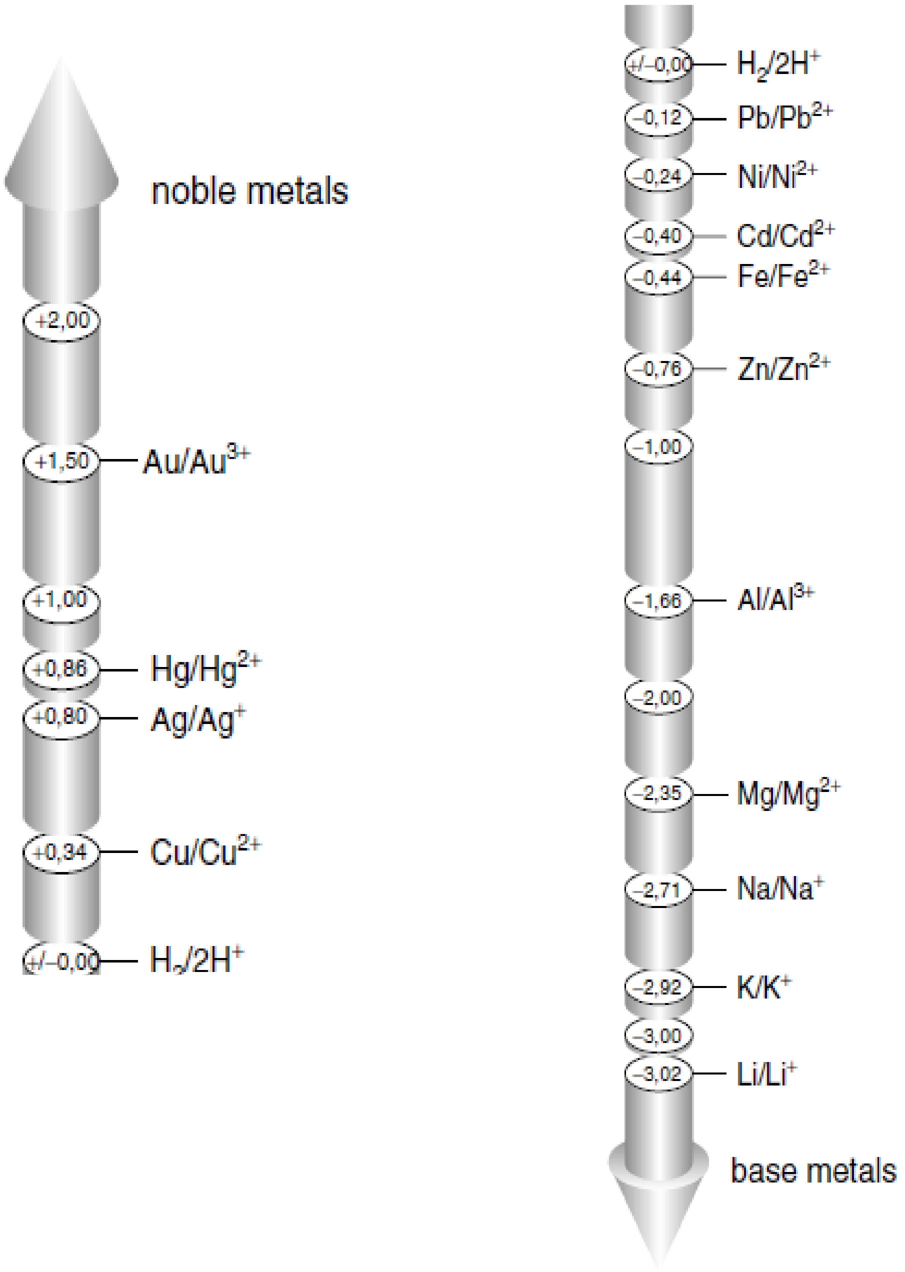
Potencial Eléctrico

Serie Electroquímica de Metales
Potencial Standard



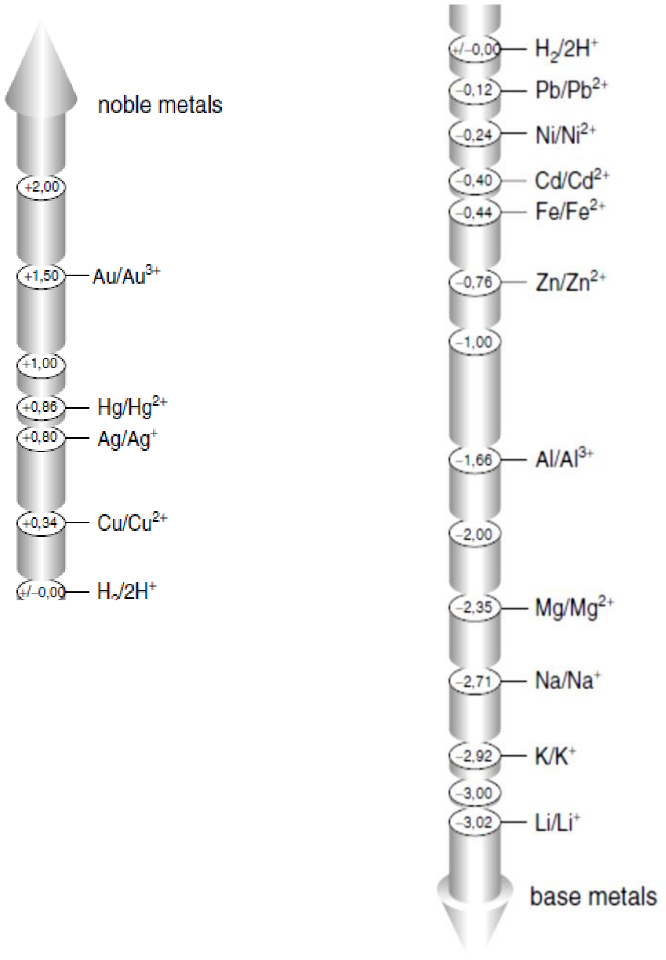


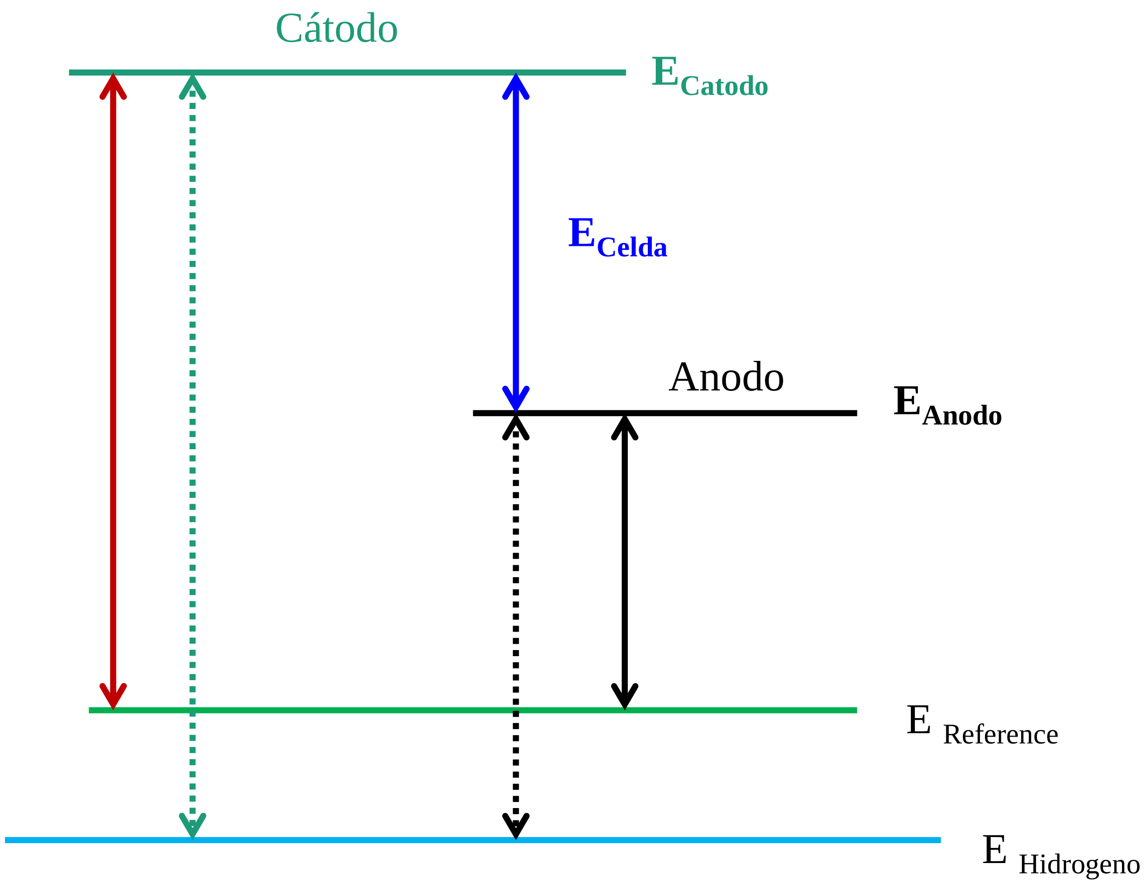
- Voltage de una celda?



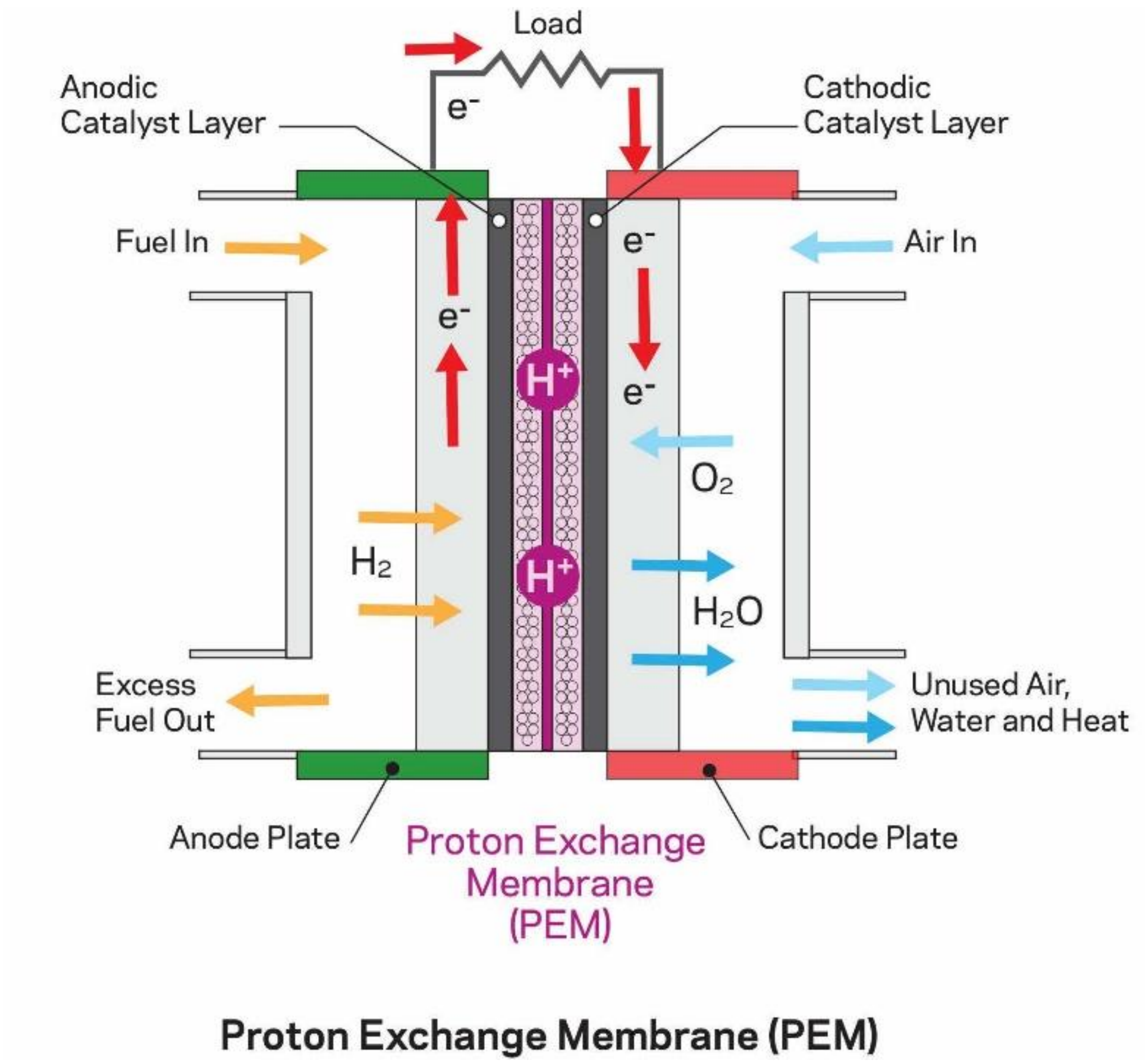
Potencial y Voltage

Voltage de una Celda





PEM Fuel Cell



Proton Exchange Membrane Fuel Cell

Anode: $H_2(g) \rightarrow 2H^+(aq) + 2e^-$

Cathode: $\frac{1}{2}O_2(g) + 2H^+(aq) + 2e^- \rightarrow H_2O$

Overall: $H_2(g) + \frac{1}{2}O_2(g) + x_w H_2O \rightarrow (x_w + 1)H_2O$

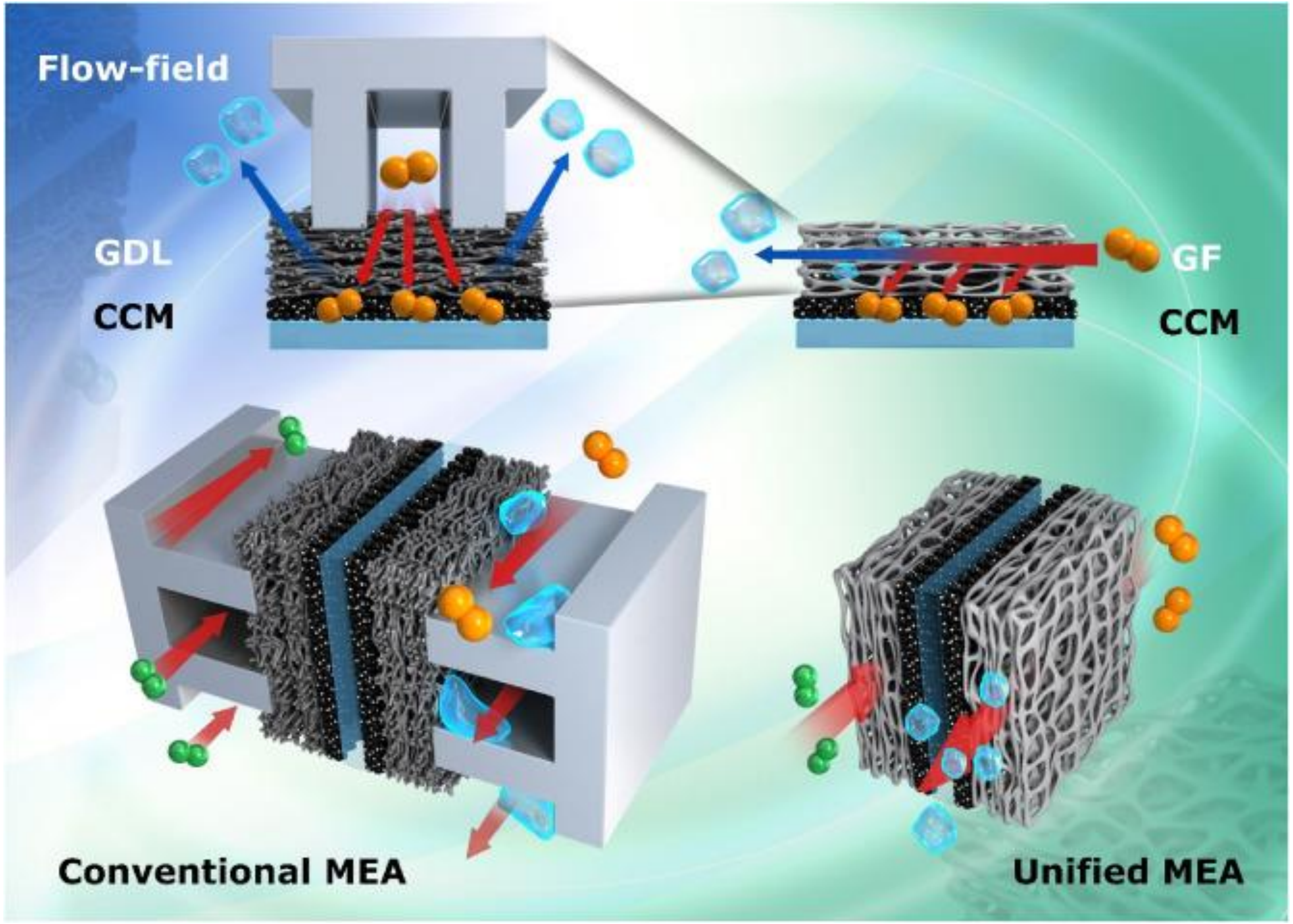
CCM = Catalyst Coated Membrane
MEA = Membrane – Electrode – Assembly
GDL = Gas Difussion Layer
GF = Gas Flow

CF = Grafito

GDL = Carbon

E = Carbon + Platino

M = Polímero PTFE



MEA (Membrane Electrode Assembly)

Corriente Eléctrica

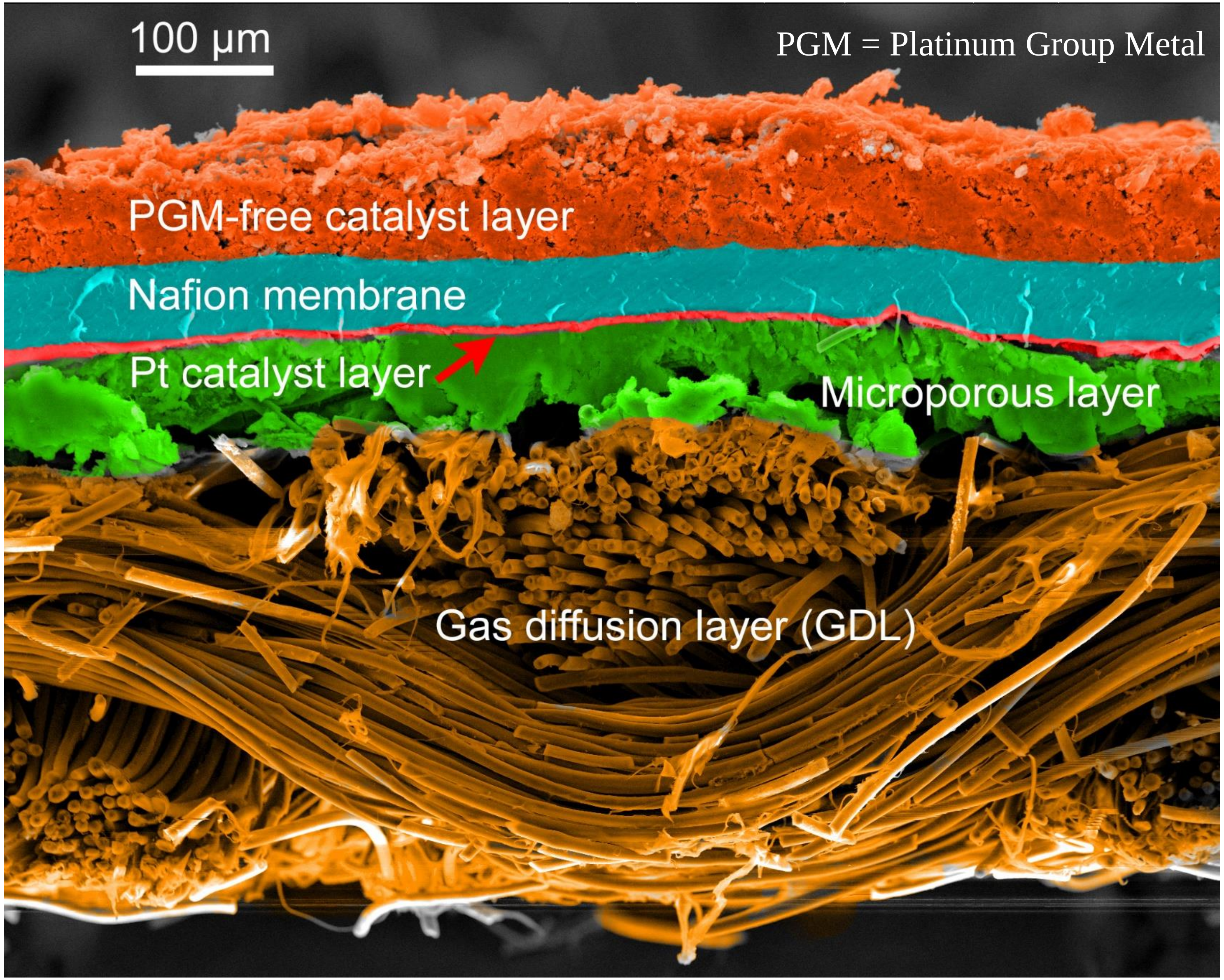
Diferencia de Potencial

Carga Eléctrica

$$F = 96485 \frac{J}{V \cdot mol\ e^-}$$

$$\Delta G = -nFE$$

Reacciones

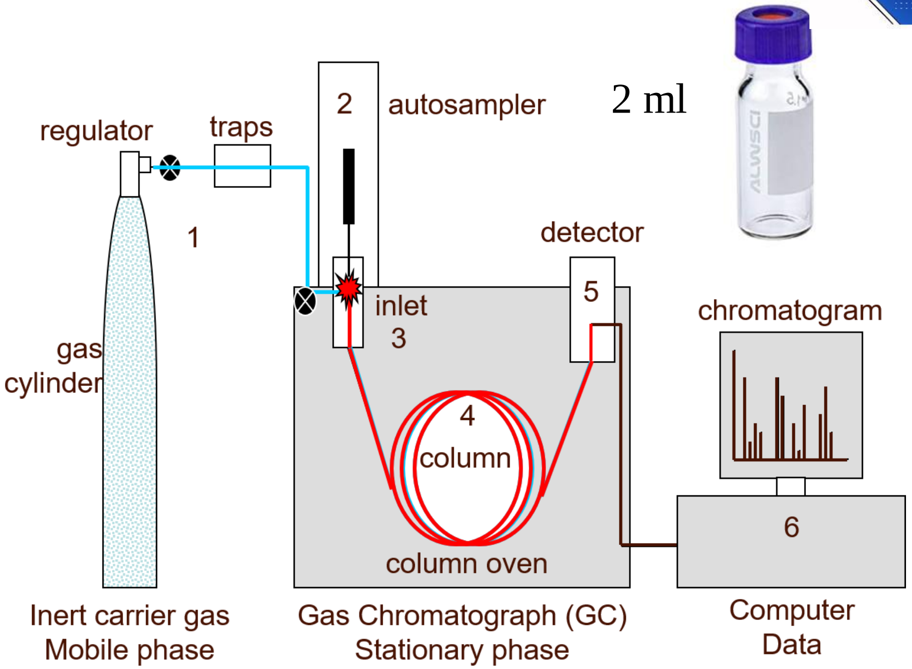


Materials

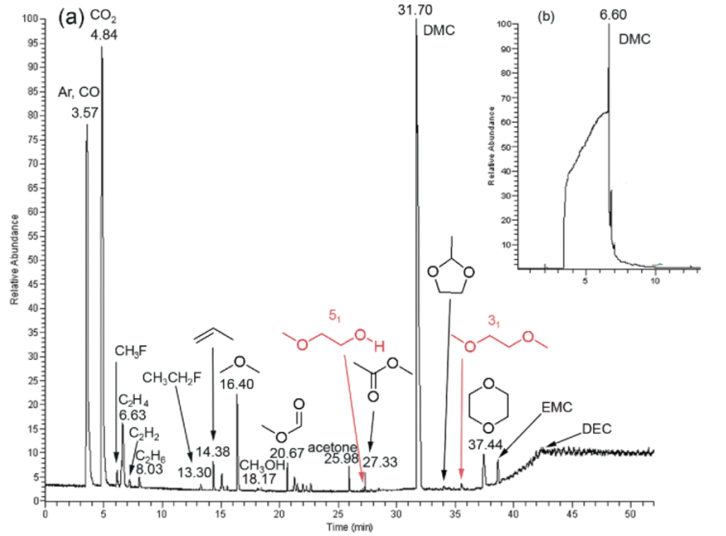
Chemical Properties – Liquid and Gases

(GC-MS) Gas Chromatography – Mass Spectrometry

Mix of liquid and gases → Composition?



2 ml

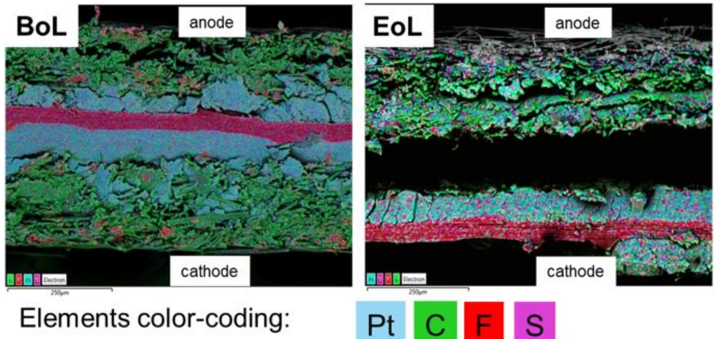


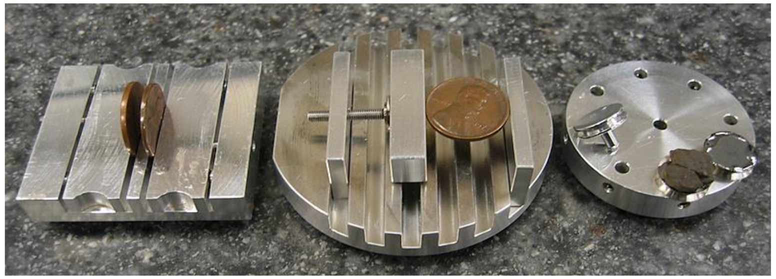
3. (a) "Gas" GC/MS and (b) "liquid" GC/MS (dilution in acetonitrile) chromatograms of the EC-DMC/$LiPF_6$ electrolyte recov

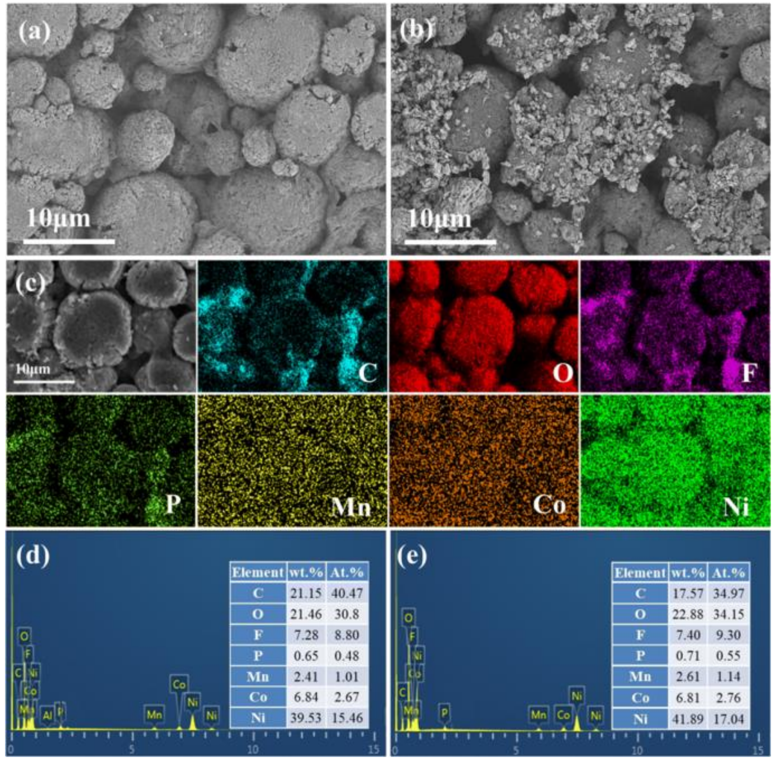
Materials

Chemical Properties – Solid

Energy-dispersive X-ray spectroscopy (XDS or EDS)







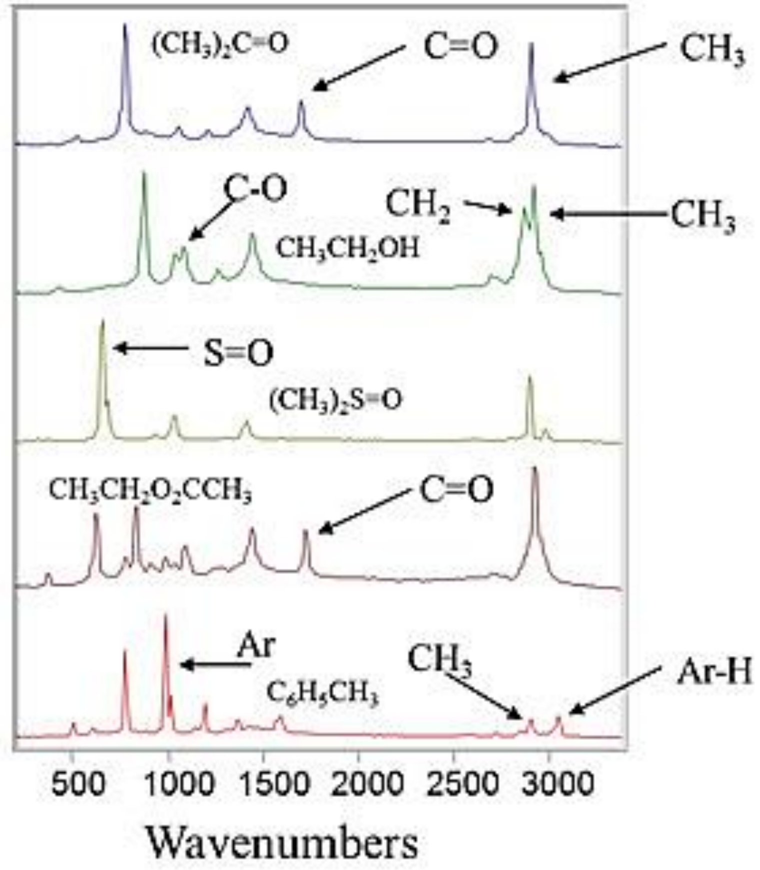
Materials

Chemical Properties – Solid

Raman spectroscopy

- Estructura química
- Fase
- Polimorfia
- Cristalinidad
- Molecular interacciones

Figure R-1 Example Raman Spectra of Various Molecules



Materials

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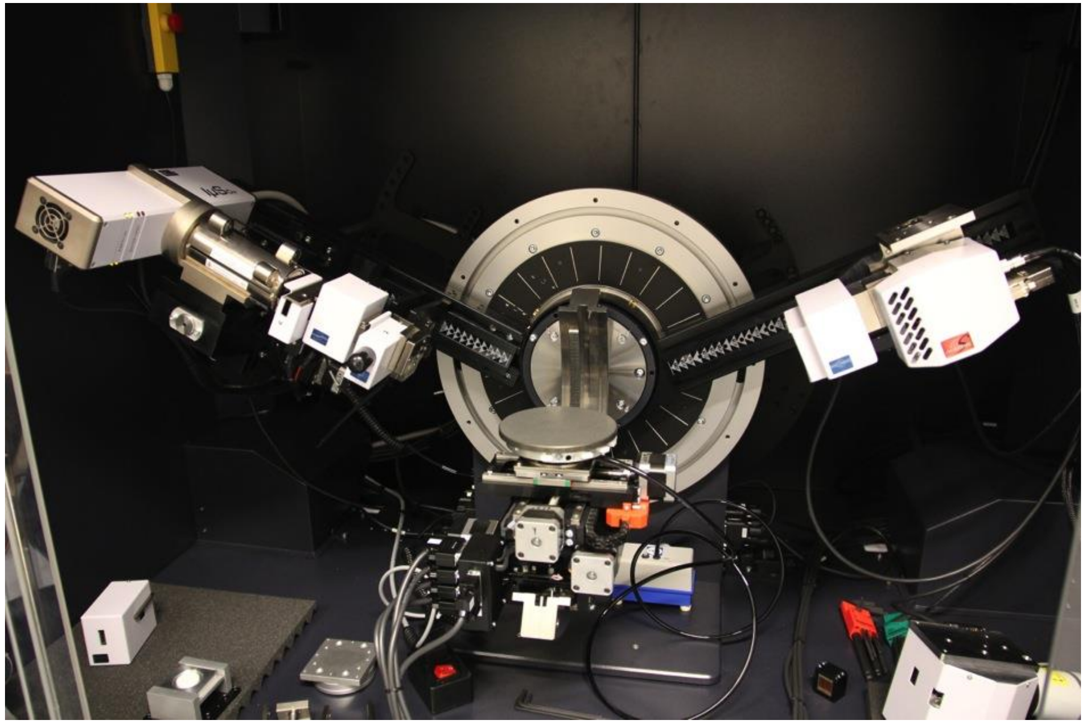
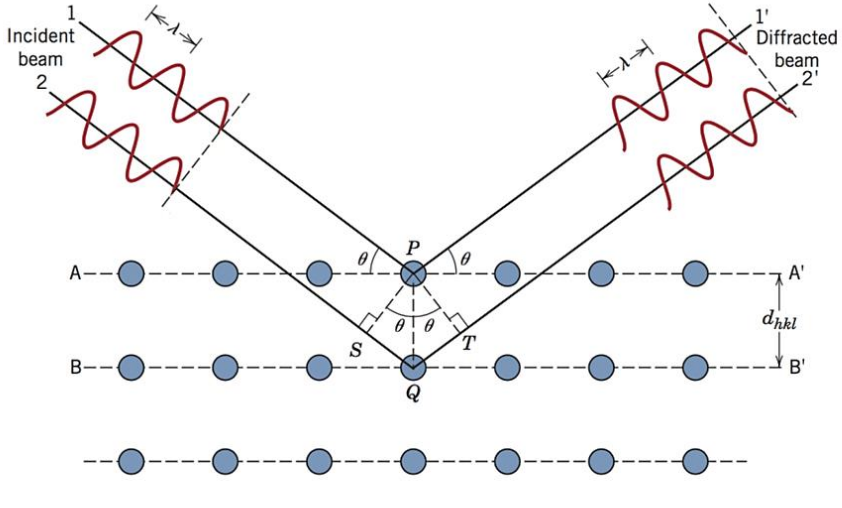
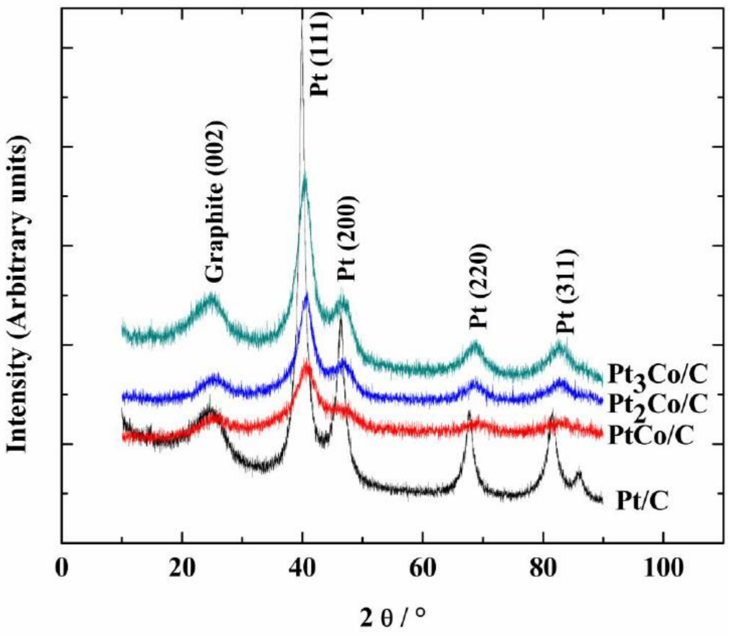
Chemical Properties – Solid

X-ray diffraction analysis (XRD) spectroscopy





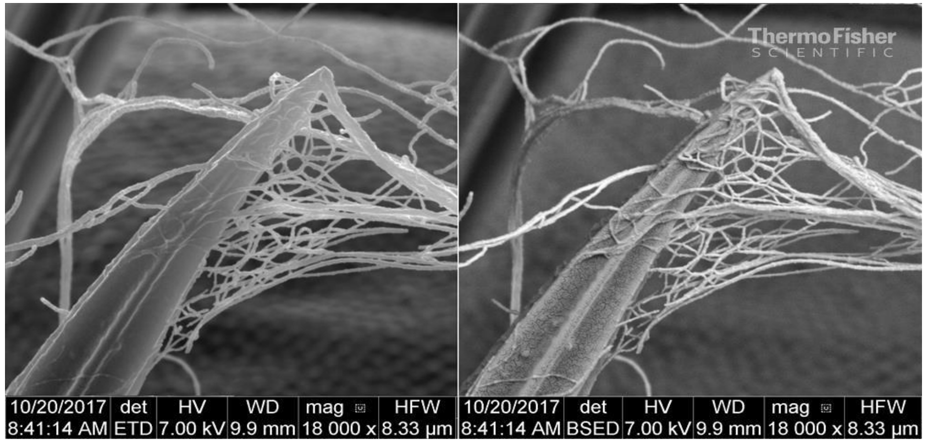
- Estructura cristalina
- Fases cristalinas
- Composición química

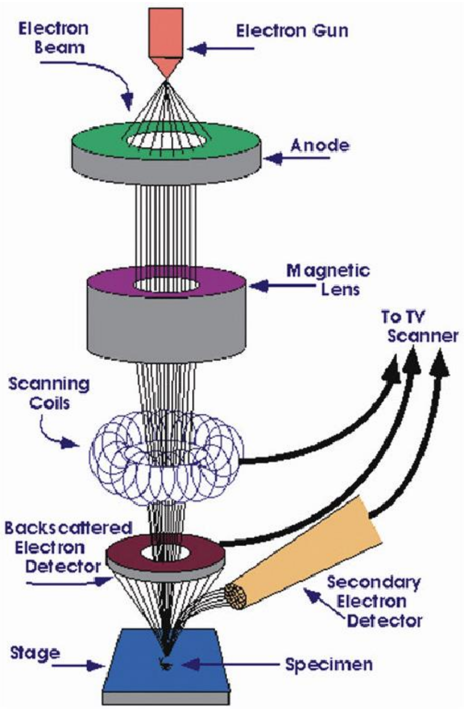


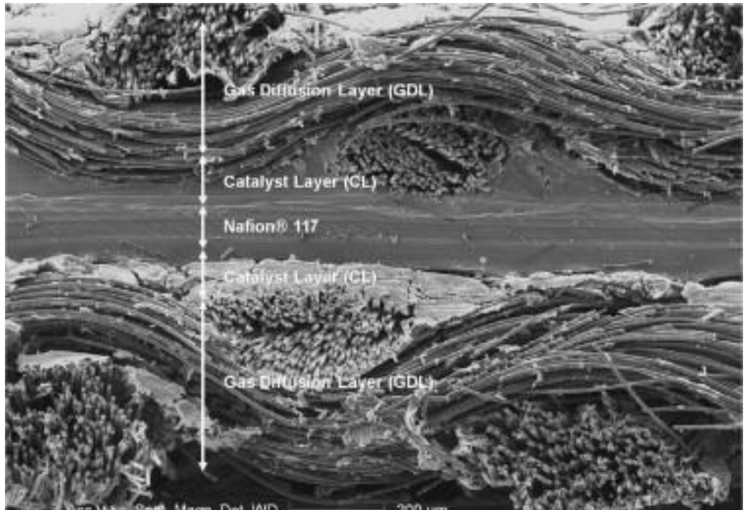
Materials

Morphology

Scanning Electron Microscopy (SEM)

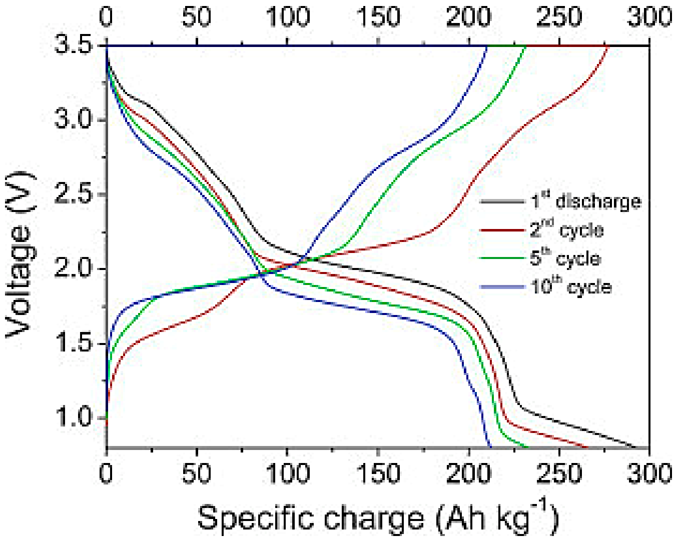


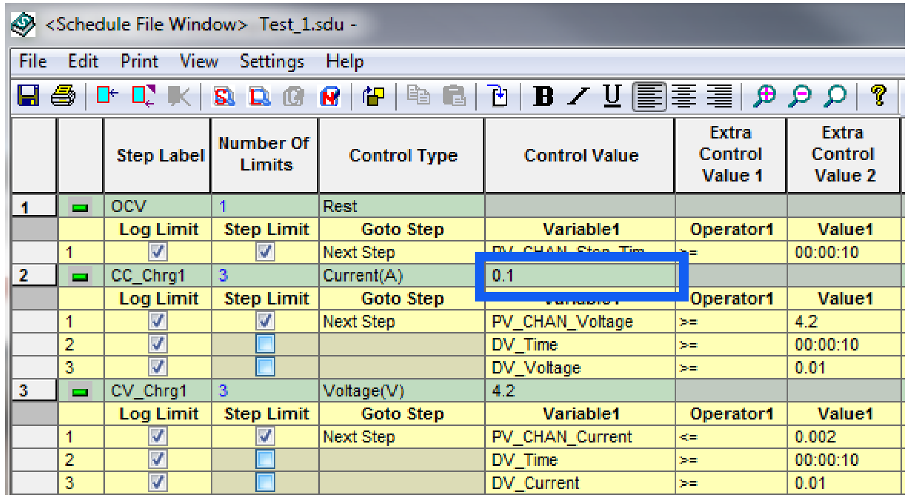




Electrochemical

Cycling / Performance / Charge-Discharge





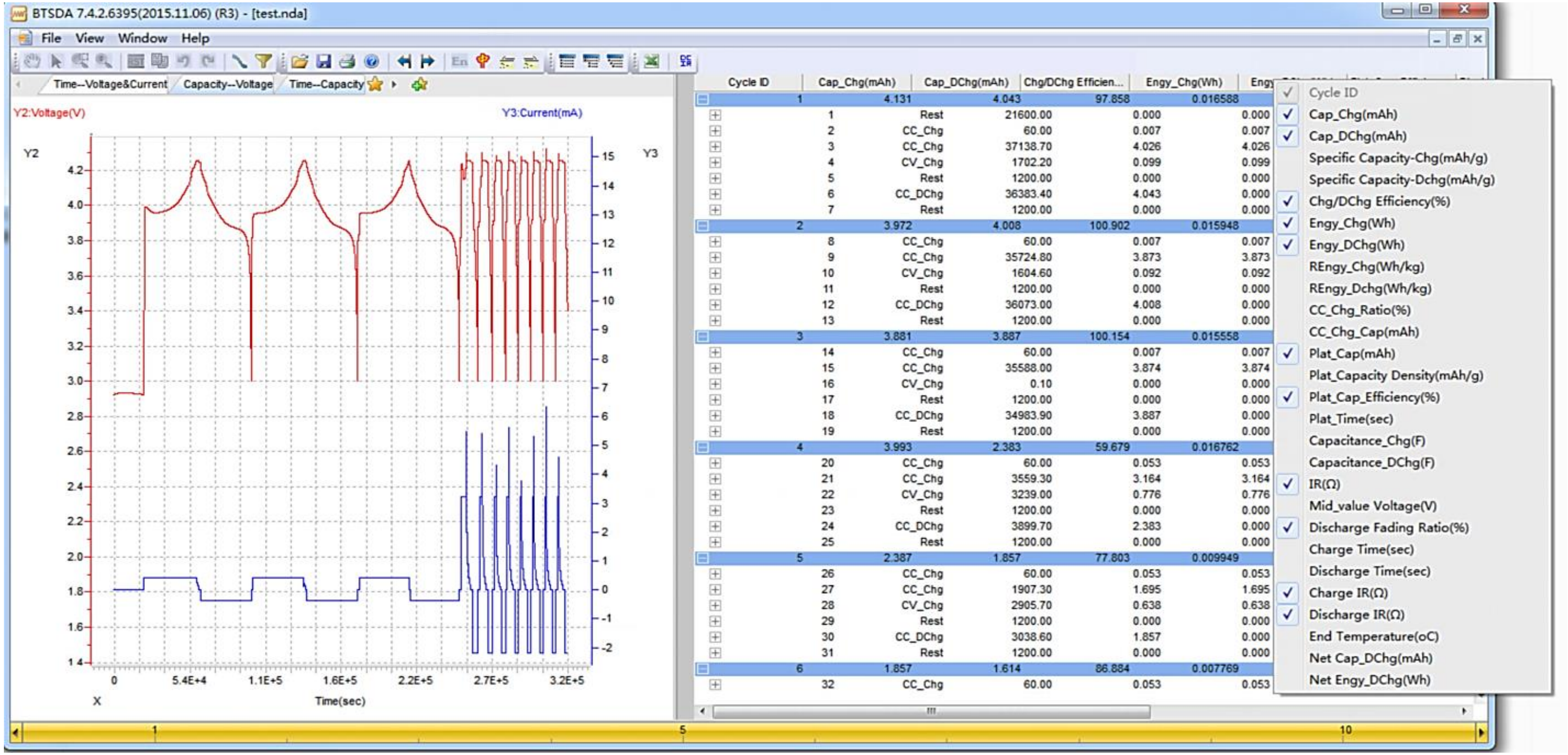
		Step Label	Number Of Limits	Control Type	Control Value	Extra Control Value 1	Extra Control Value 2
1		OCV	1	Rest			
		Log Limit	Step Limit	Goto Step	Variable1	Operator1	Value1
	1	✓	✓	Next Step	PV_CHAN_Step_Tim	>=	00:00:10
2		CC_Chrg1	3	Current(A)	0.1		
		Log Limit	Step Limit	Goto Step	Variable1	Operator1	Value1
	1	✓	✓	Next Step	PV_CHAN_Voltage	>=	4.2
	2	✓	☐		DV_Time	>=	00:00:10
	3	✓	☐		DV_Voltage	>=	0.01
3		CV_Chrg1	3	Voltage(V)	4.2		
		Log Limit	Step Limit	Goto Step	Variable1	Operator1	Value1
	1	✓	✓	Next Step	PV_CHAN_Current	<=	0.002
	2	✓	☐		DV_Time	>=	00:00:10
	3	✓	☐		DV_Current	>=	0.01

Battery Tester

Fuente de Poder

Electrochemical

Cycling / Performance / Charge-Discharge

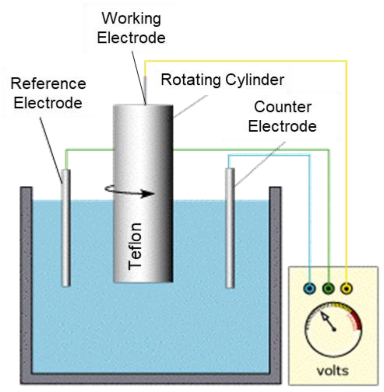


Electrochemical

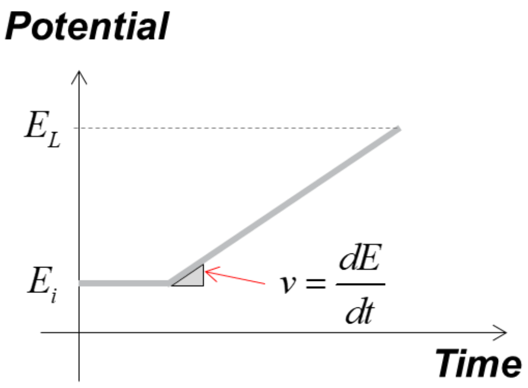
Cyclic Voltammetry

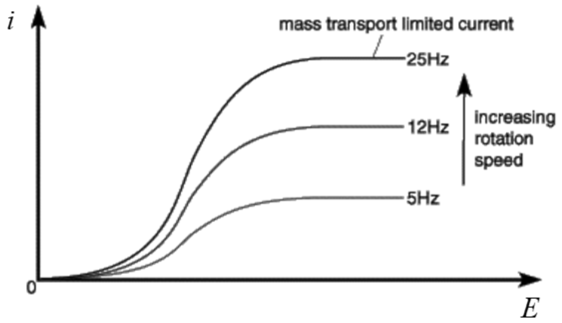
- Cyclic voltammetry (CV) is the most widely used technique for acquiring qualitative information about electrochemical reactions. CV provides information about:
- Redox processes, Heterogeneous electron – transfer reactions, Adsorption processes

Linear Sweep Voltammetry (LSV)



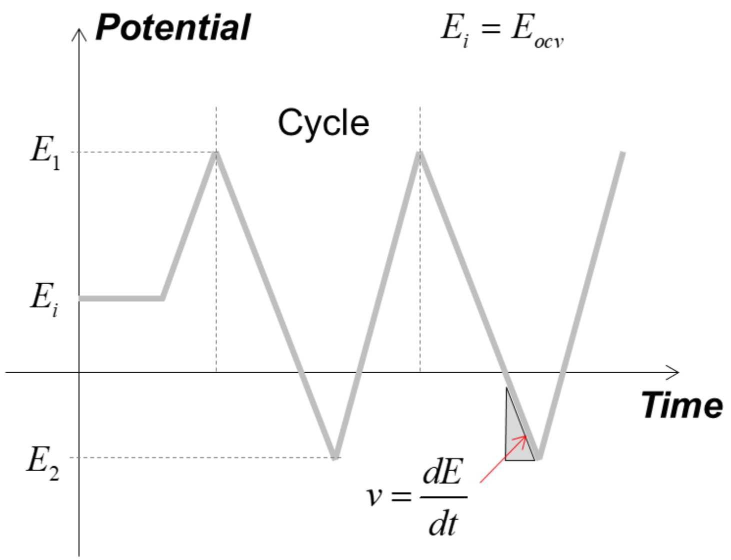
Mass transport limited current as a function of the rotation speed by Levich





$$i_L = 0.62nFAC_{Bulk}D^{2/3}\nu^{-1/6}\omega^{1/2}$$

Cyclic Voltammetry (CV)



$$\frac{dE}{dt} = (2N)\left(\frac{E_1 - E_2}{t_{Total}}\right) \Rightarrow t_{Total} = (2N)\left(\frac{E_1 - E_2}{dE/dt}\right)$$

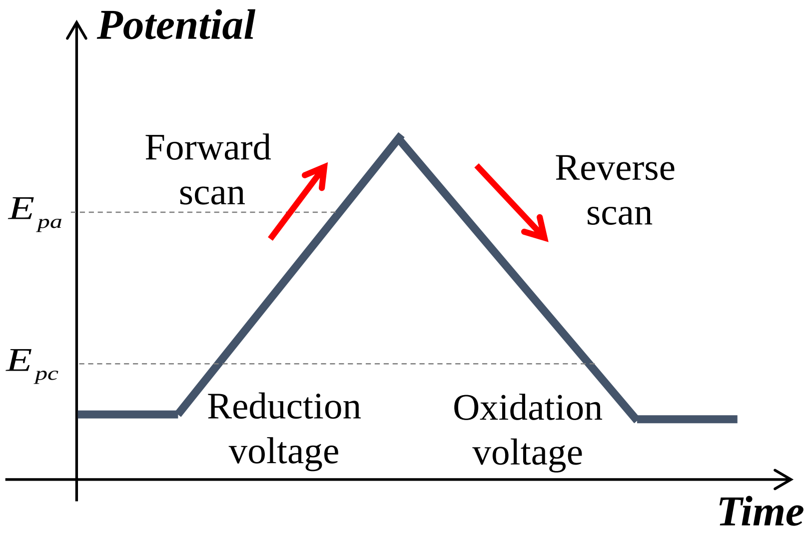
Electrochemical

CV - Anodic and Cathodic Current

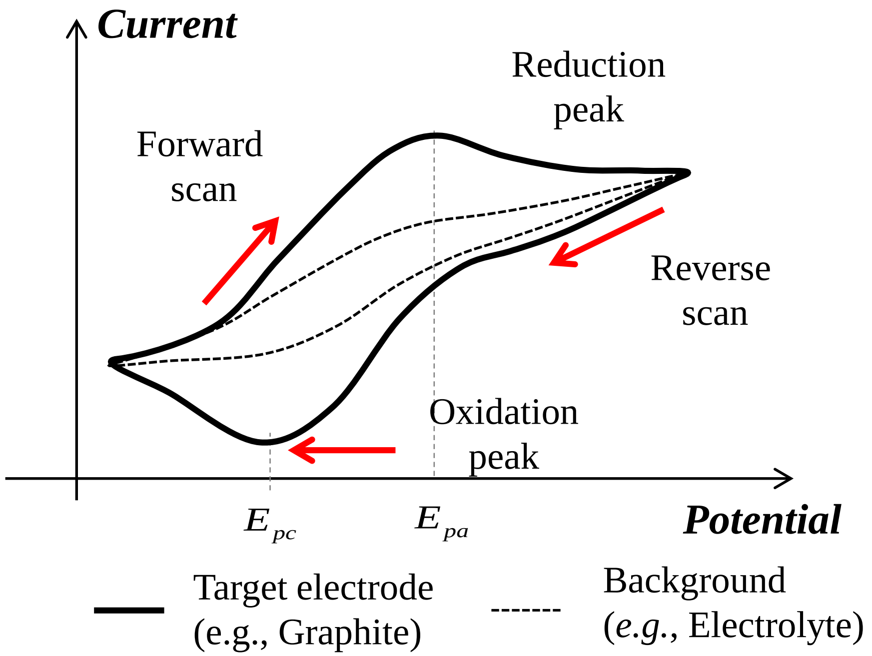
Direction of the Process and Sign Convention

American
- Cathodic current positive
- Negative potentials decreasing to the right

IUPAC (International Union of Pure and Applied Chemistry)
- Anodic currents positive
- Positive potentials increasing to the right



$$Li_xC \xrightleftharpoons[\text{charge}]{\text{discharge}} C + xLi^+ + xe^-$$



Electrochemical

CV - Irreversible Systems

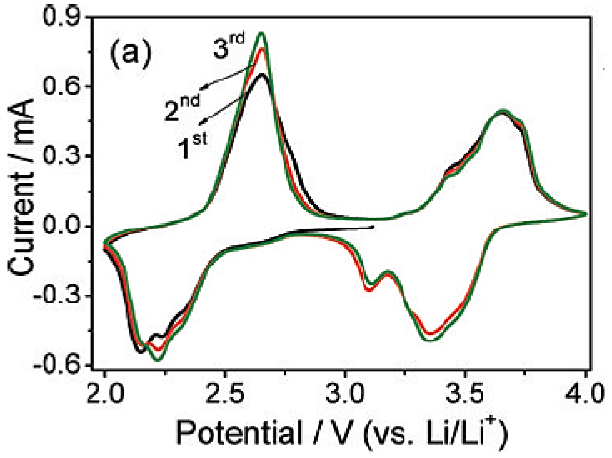
Vanadium pentoxide (Carbon-coated V_2O_5 nanocrystalls) exhibits different phases based on the operating voltage window.

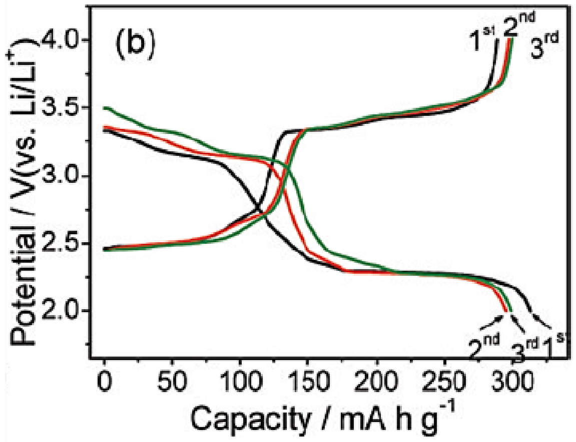
$$\alpha - V_2O_5 + \frac{1}{2}Li^+ + \frac{1}{2}e^- \rightleftharpoons \varepsilon - Li_{0.5}V_2O_5$$

$$\varepsilon - Li_{0.5}V_2O_5 + \frac{1}{2}Li^+ + \frac{1}{2}e^- \rightleftharpoons \delta - LiV_2O_5$$

$$\delta - LiV_2O_5 + Li^+ + e^- \rightleftharpoons \gamma - Li_2V_2O_5$$

Phase	$Li_xV_2O_5$
α - phase	x < 0.01
ε - phase	0.35 < x < 0.7
δ - phase	0.7 < x < 1.0
γ - phase	1.0 < x < 2.0
ω - phase	2.0 < x < 3.0





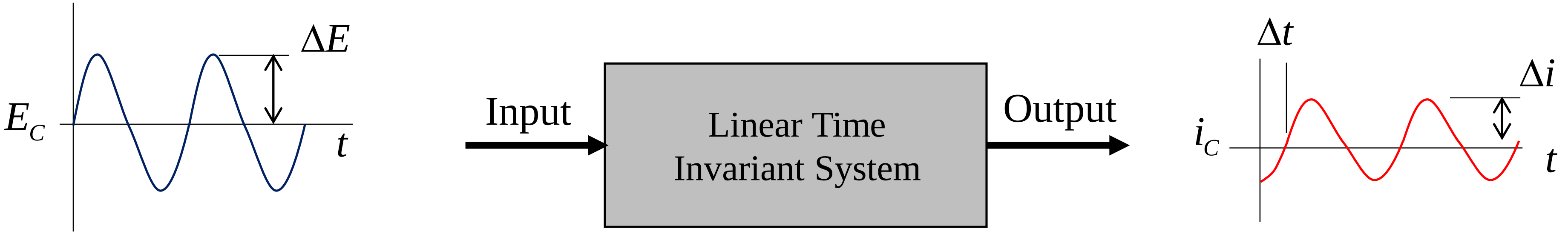
Cyclic voltammograms at a scan rate of 1.0 mV/s and (b) the first three discharge-charge profiles recorded at 1.0 A/g for the carbon-coated V_2O_5.

Zhang et al., Chem. Mater. 2011, 23, 5290-5292

Electrochemical

EIS – Impedance Measurement

Electrochemical Impedance is usually measured by applying an AC potential (Potentiostatic) to an electrochemical cell and then measuring the current through the cell.



$$E(t) = E_C + \Delta E \, Sin(\omega t)$$

$$\omega = 2\pi f$$

$$i(t) = i_C + \Delta i \, Sin(\omega t - \phi)$$

Laplace Transform

$$F(s) = \mathcal{L}\{f(t)\} = \int_{-\infty}^{\infty} e^{-st} f(t) \, dt$$

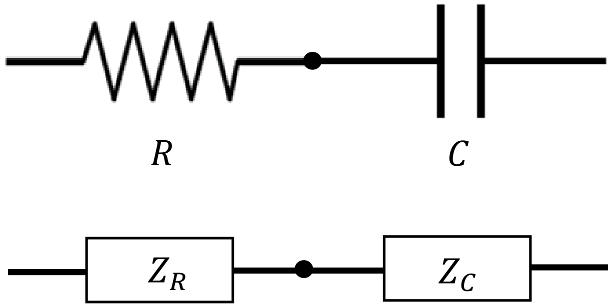
$$s = j\omega$$

$$j = \sqrt{-1}$$

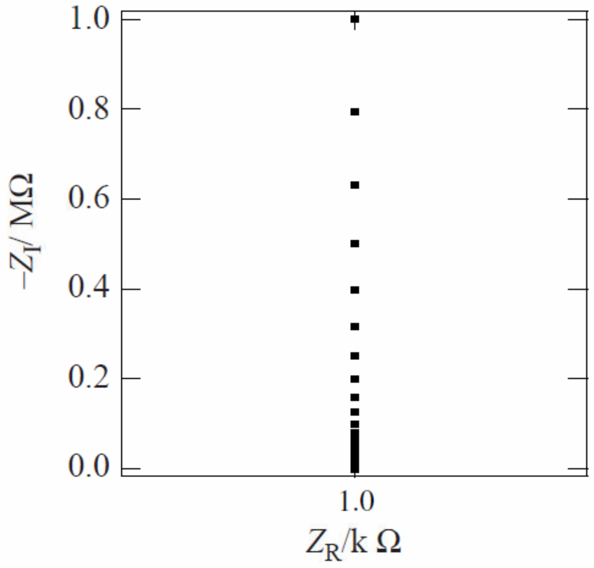
Electrochemical

EIS – Two Phase Circuit (RC)

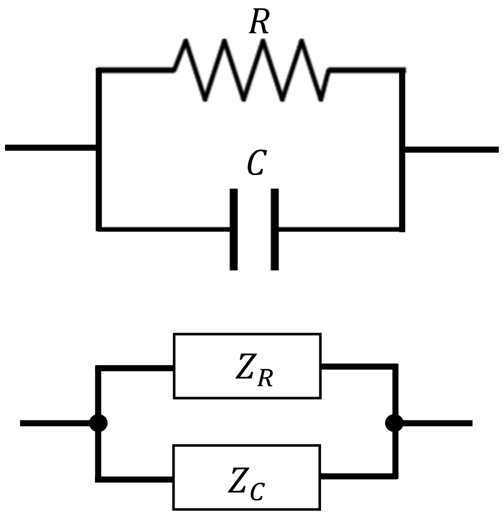
Serial RC circuit



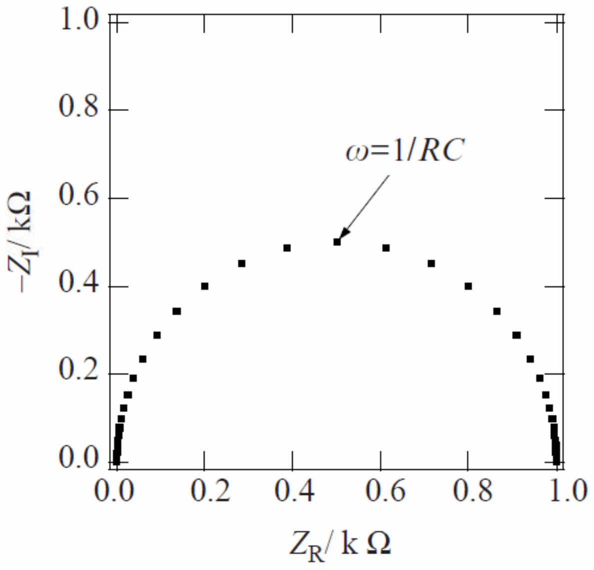
$$Z(\omega) = Z_R(\omega) + Z_C(\omega)$$
$$= R + \frac{1}{j\omega C}$$
$$|Z(\omega)| = \sqrt{R^2 + \left(-\frac{1}{\omega C}\right)^2}$$



Parallel RC circuit

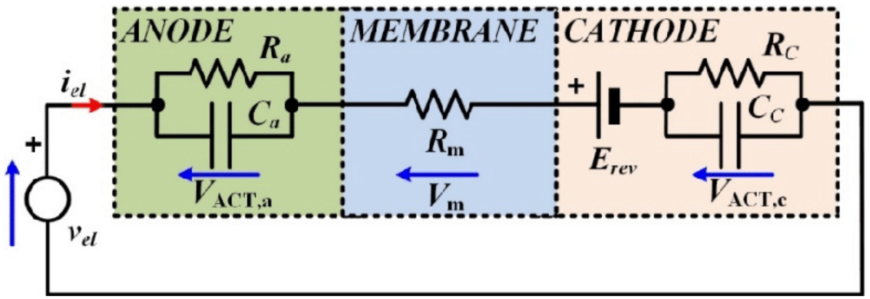


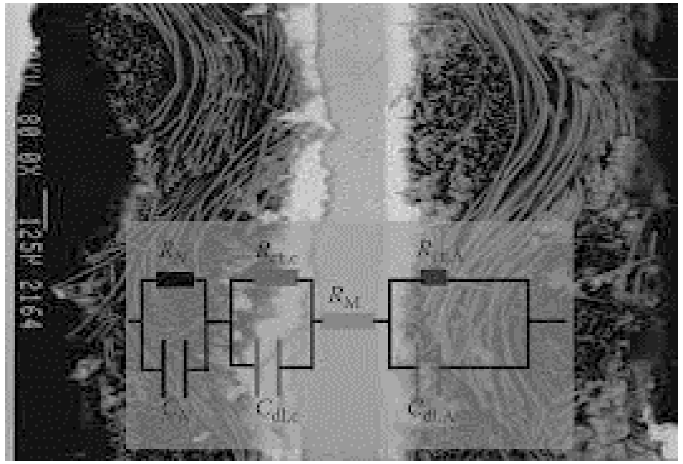
$$\frac{1}{Z(\omega)} = \frac{1}{Z_R(\omega)} + \frac{1}{Z_C(\omega)}$$
$$= \frac{1}{R} + j\omega C = \frac{1 + Rj\omega C}{R}$$
$$Z(\omega) = \frac{R}{1 + Rj\omega C}$$
$$|Z(\omega)| = \sqrt{\left(\frac{1}{R}\right)^2 + (\omega C)^2}$$

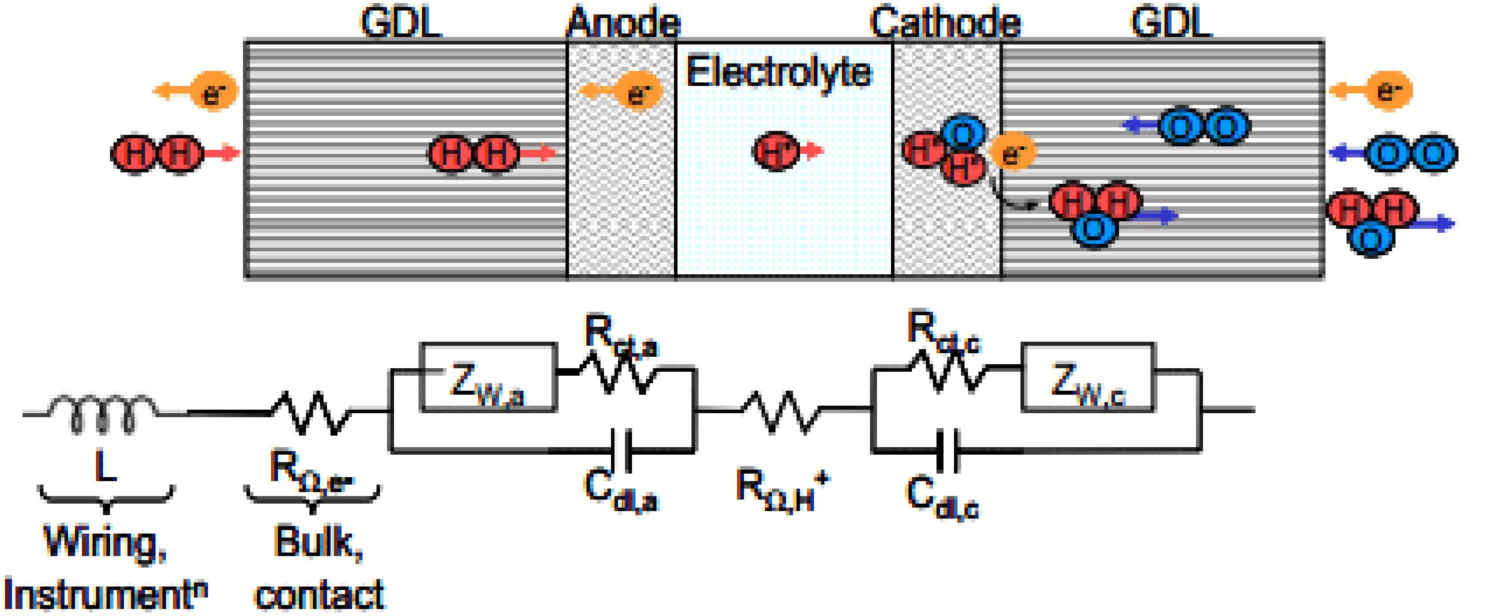


Electrochemical

EIS – PEMFC Equivalent Circuit





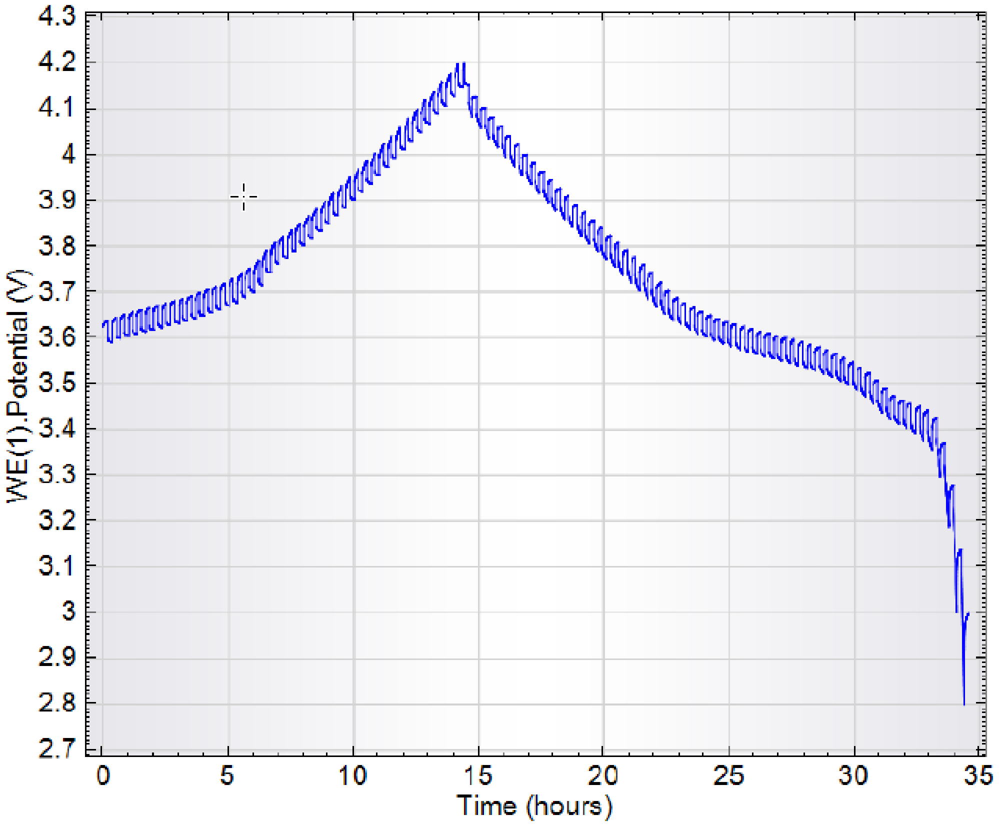


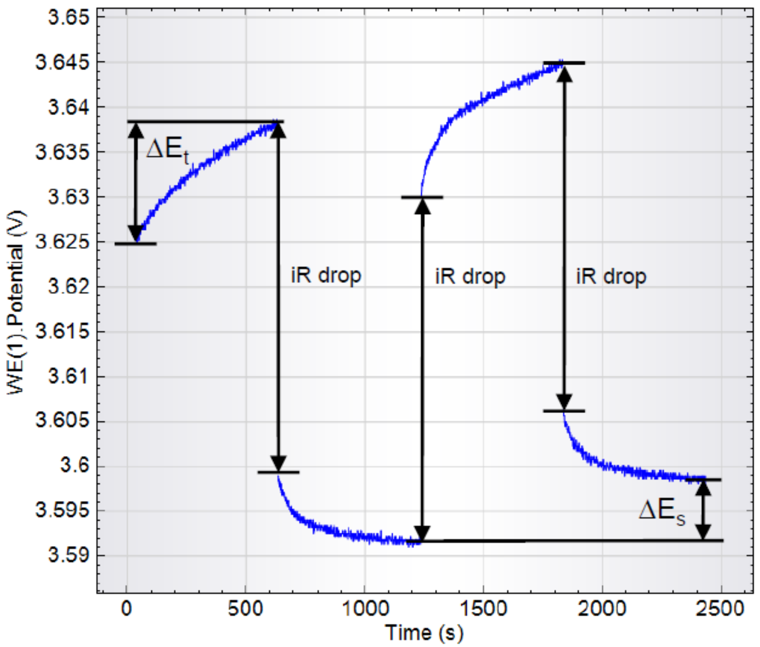
Key: GDL = gas diffusion layer, dl = double layer, ct = charge transfer, a = anode, c = cathode.

Electrochemical

GITT - Galvanostatic Intermittent Titration Technique

The galvanostatic intermittent titration technique (GITT) is a procedure useful to retrieve both thermodynamics and kinetics parameters





$$D = \frac{4}{\pi}\left(\frac{iV_m}{z_A F S}\right)^2 \left[\left(dE/_{d\delta}\right) \Big/ \left(dE/_{d\sqrt{t}}\right)\right]^2$$

$$D = \frac{4}{\pi\tau}\left(\frac{n_m V_m}{S}\right)^2 \left(\frac{\Delta E_s}{\Delta E_t}\right)^2$$

Thermal

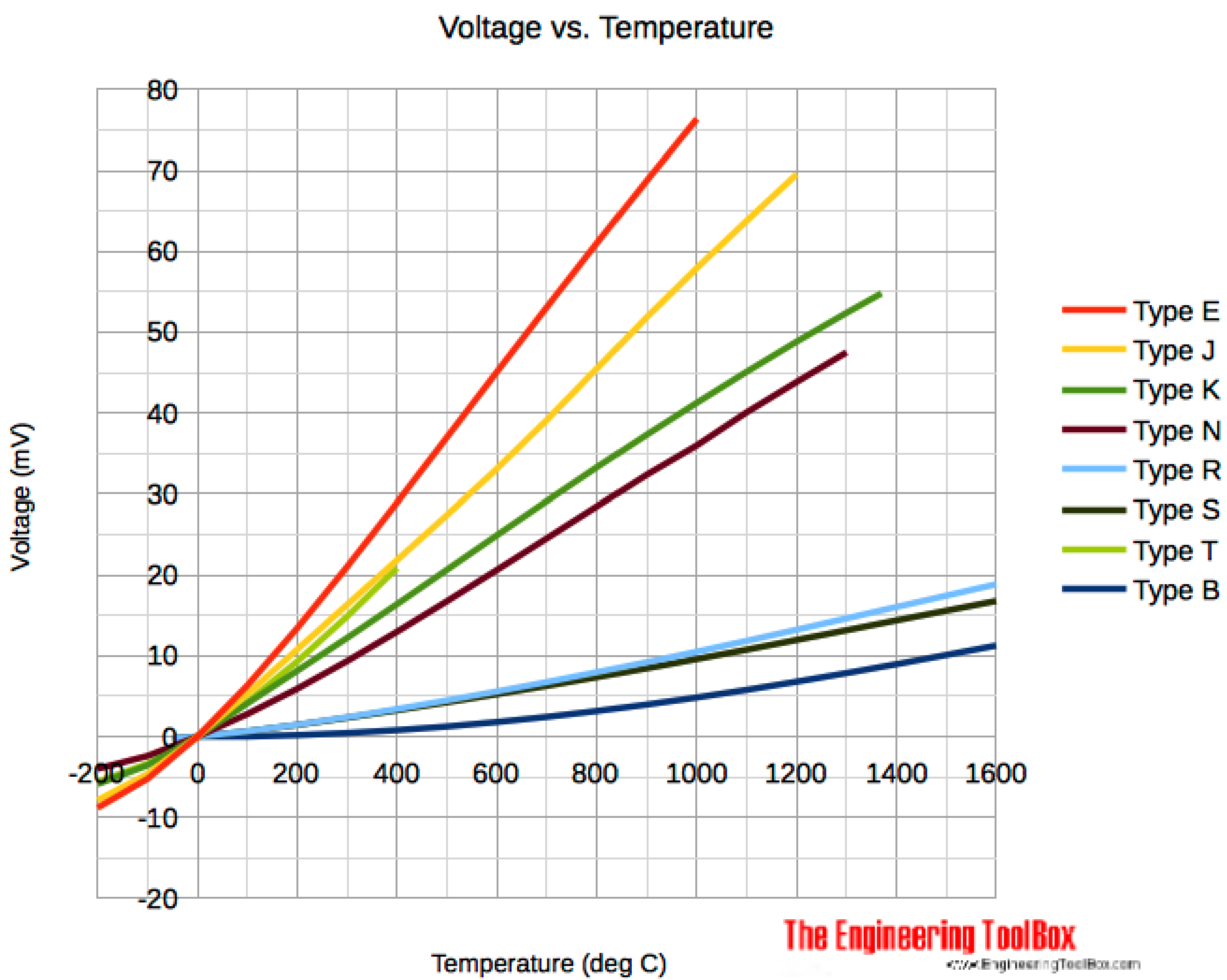
Temperature

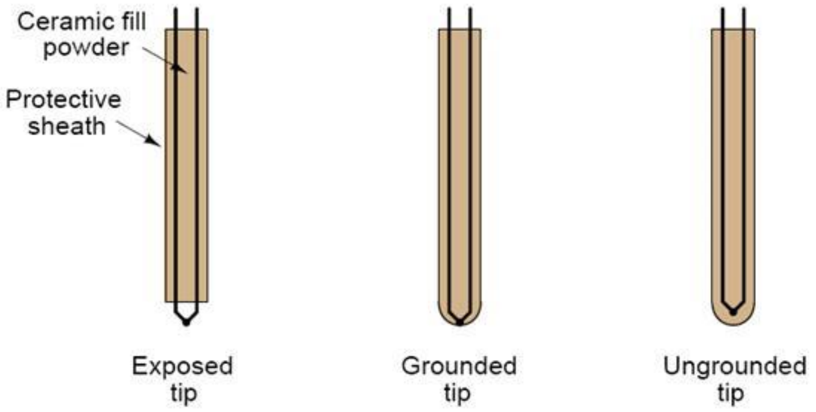
THERMOCOUPLE CHARACTERISTICS TABLE

ANSI/ASTM	Symbol Single	Generic Names	Color Coding: Individual Conductor	Color Coding: Overall Jacket Extension Grade Wire	Magnetic Yes/No	Environment (Bare Wire)
T	TP TN	Copper Constantan, Nominal Composition: 55% Cu, 45% Ni	Blue Red	Blue	No No	Mild Oxidizing, Reducing. Vacuum or Inert. Good where moisture is present.
J	JP JN	Iron Constantan, Nominal Composition: 55% Cu, 45% Ni	White Red	Black	Yes No	Reducing Vacuum, Inert. Limited use in oxidizing at High Temperatures. Not recommended for low temps.
E	EP EN	Chromel®, Nominal Composition: 90% Ni, 10% Cr Constantan, Nominal Composition: 55% Cu, 45% Ni	Purple Red	Purple	No No	Oxidizing or Inert. Limited use in Vacuum or Reducing.
K	KP KN	Chromel, Nominal Composition: 90% Ni, 10% Cr Alumel®, Nominal Composition: 95% Ni, 2% Mn, 2% Al	Yellow Red	Yellow	No Yes	Clean Oxidizing and Inert. Limited use in Vacuum or Reducing
N	NP NN	Nicrosil®, Nominal Compositions: 84.6% Ni, 14.2% Cr, 1.4% Si Nisil®, Nominal Composition: 95.5% Ni, 4.4% Si, 1% Mg	Orange Red	Orange	No No	Clean Oxidizing and Inert. Limited use in Vacuum or Reducing
S	SP SN	Platinum 10% Rhodium Pure Platinum	Black Red	Green	No No	Oxidizing or Inert Atmospheres. Do not insert in metal tubes. Beware of contamination.
R	RP RN	Platinum 13% Rhodium Pure Platinum	Black Red	Green	No No	Oxidizing or Inert Atmospheres. Do not insert in metal tubes. Beware of contamination.
B	BP BN	Platinum 30% Rhodium Platinum 6% Rhodium	Gray Red	Gray	No No	Oxidizing or Inert Atmospheres. Do not insert in metal tubes. Beware of contamination.
C*	P N	Tungsten 5% Rhenium Tungsten 26% Rhenium	Green Red	Red	No No	Vacuum, Inert, Hydrogen Atmospheres. Beware of Embrittlement.

Thermal

Temperature

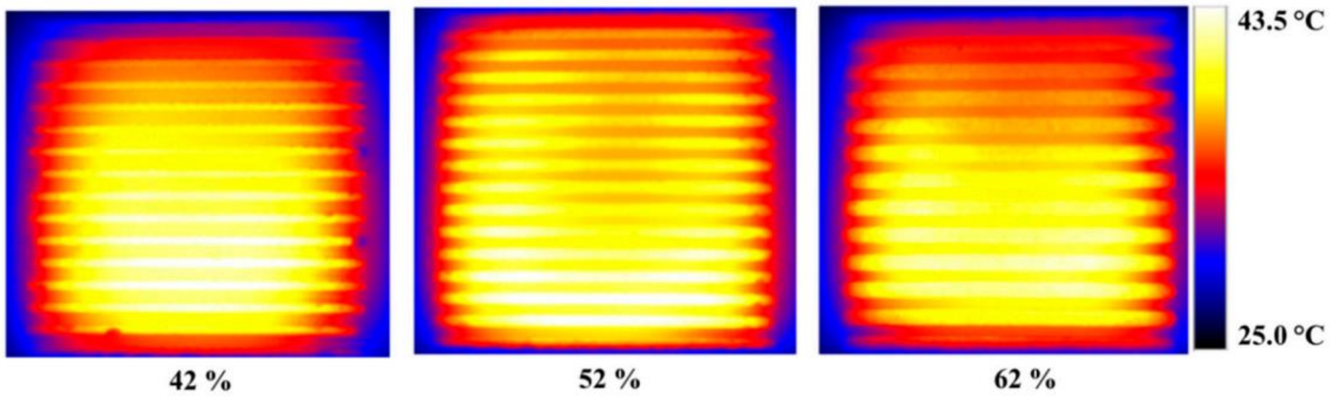




Thermal

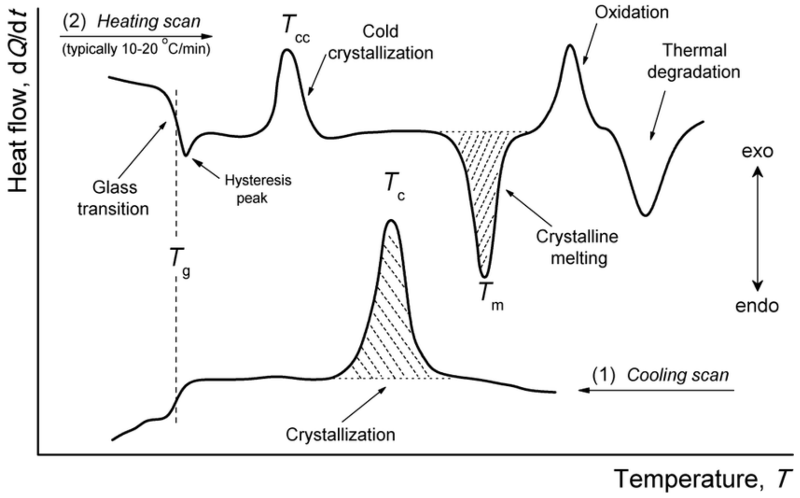
Infrared Thermal Imaging Camera

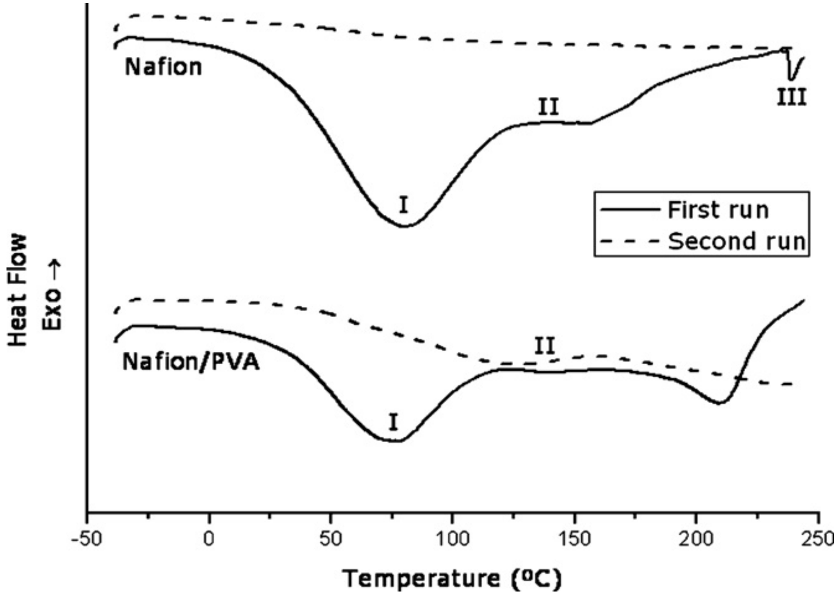
Campo de Temperatura – Fotos y Video
Análisis por medio de Procesamiento de Imágenes



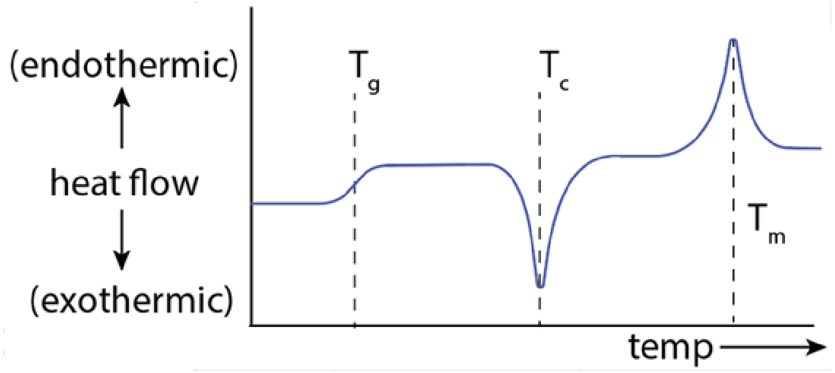
Thermal

DSC - Differential Scanning Calorimetry



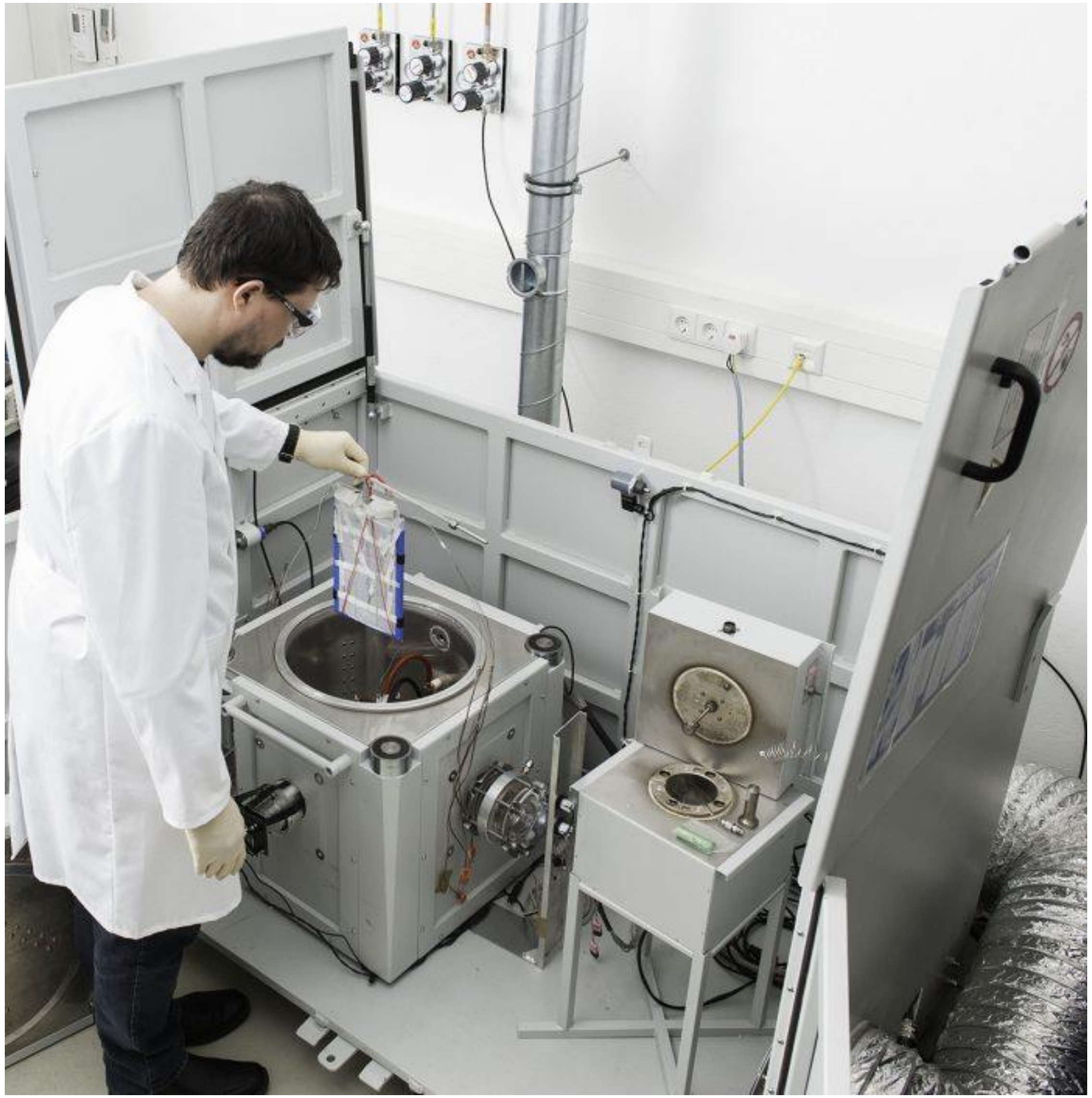


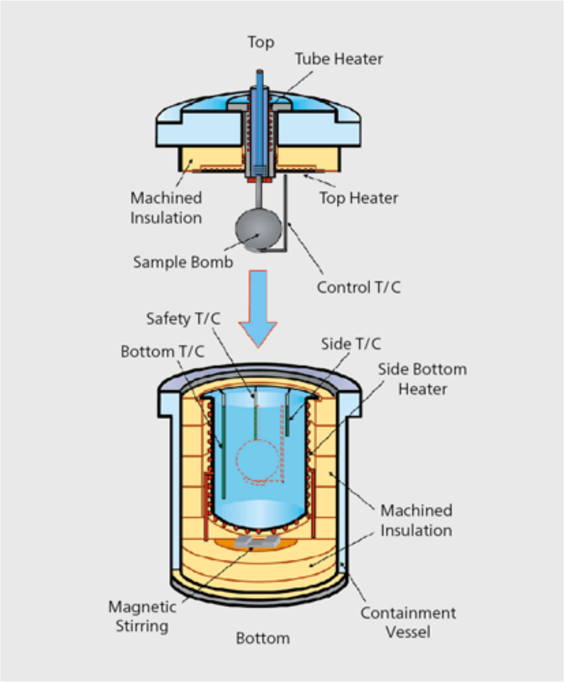
El perfil de temperatura se puede controlar.
El flujo de calor indica el tipo de reacción de la sustancia.

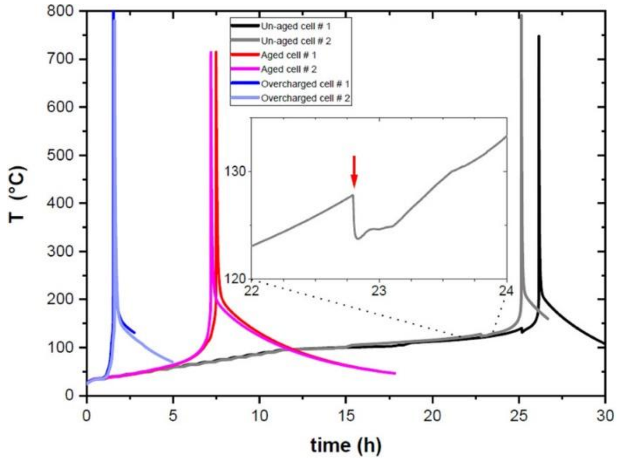


Thermal

ARC – Accelerated Rate Calorimetry





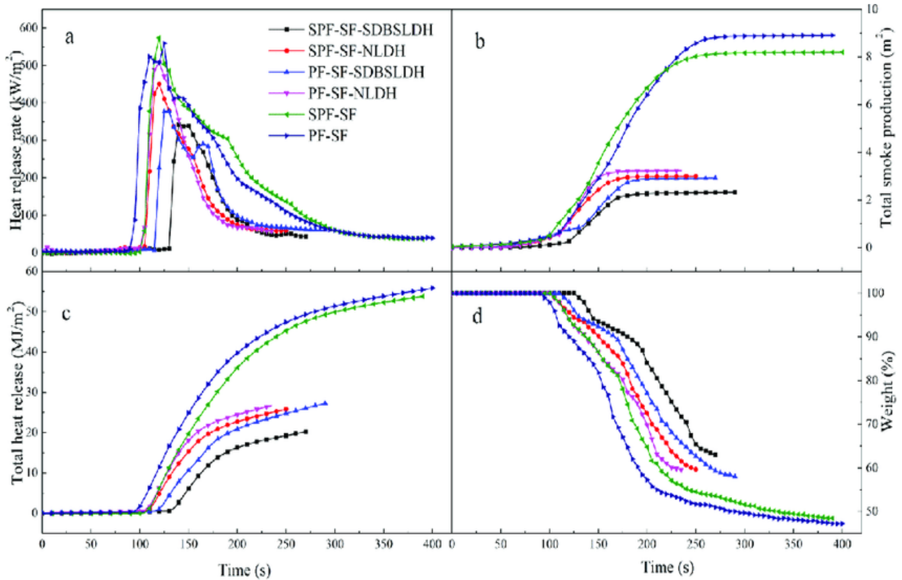


Thermal

Fire – Cone Calorimeter

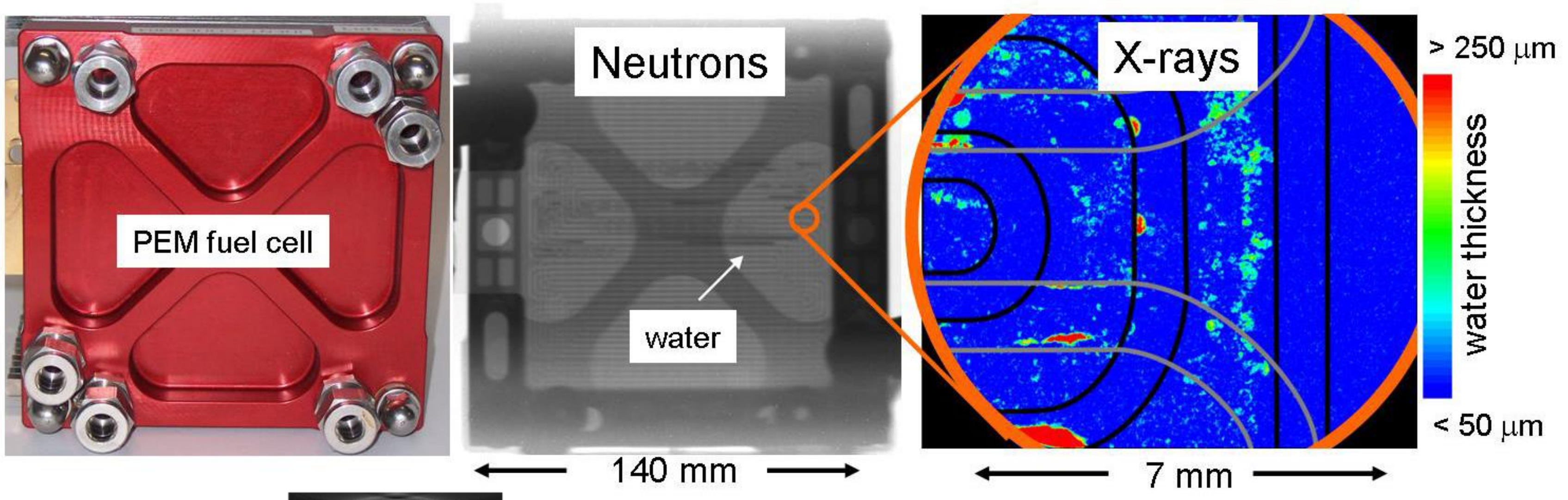
FTIR

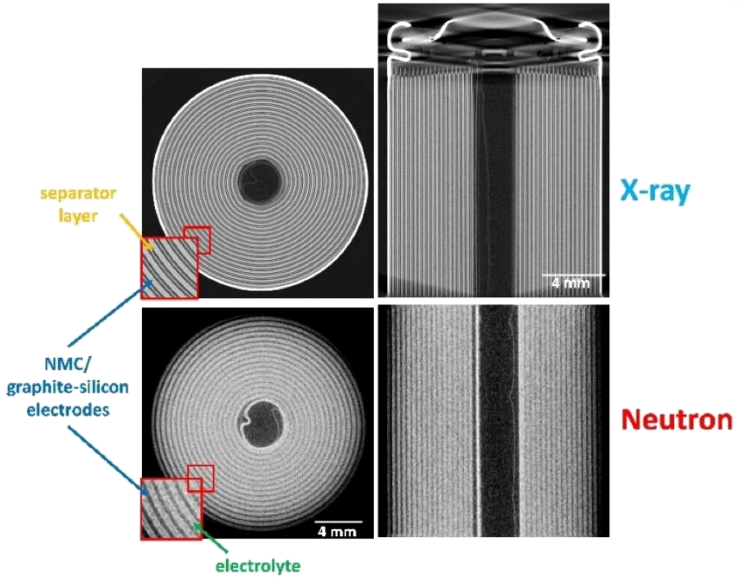
Heat release rate, Total smoke production,
Total heat release, Weight

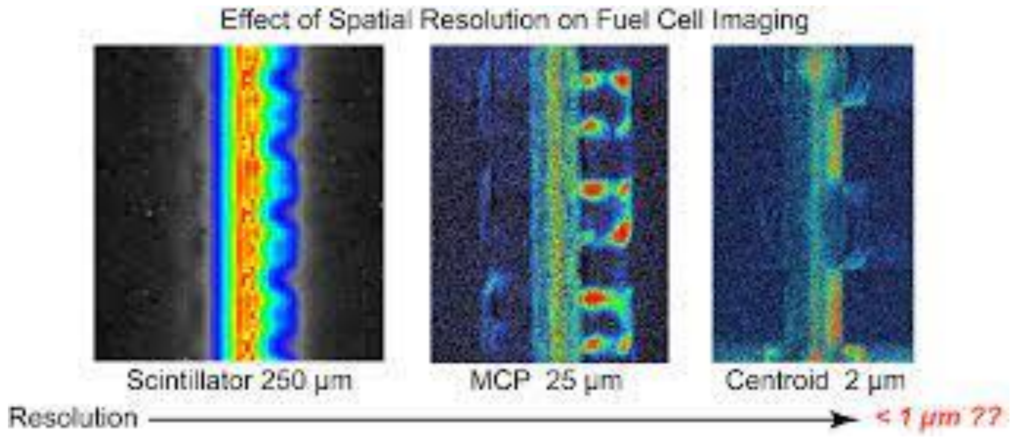


Visualization

X-ray and Neutron Diffraction Radiography







Análisis de Investigación

1. **Pregunta de Investigación.** ¿Qué fenómeno o problema quiero resolver?
2. **Revisión de Literatura.** ¿Qué análisis previos se han realizado? ¿Qué falta por analizar y considerar?
3. **Metodología.** ¿Cómo voy a analizar mi problema (Experimentos, modelos, revisión)?
4. **Variables a considerar.** ¿Qué parámetros puedo cambiar? ¿Cuáles son mis variables? ¿Qué parámetros no puedo cambiar?
5. **Recursos.** ¿Qué herramientas computacionales o experimentales tengo disponible? Colaboraciones. Tiempo.
6. **Función objetivo.** ¿De todos los parámetros o variables, cuales de ellas se relacionan directamente con mi variable objetivo? ¿En cuales de ellas me voy a enfocar? ¿ Cómo las voy a medir?
7. **Análisis de Resultados.** Post-procesamiento de datos. Inferencia de datos. Métodos heurísticos. Repetición de pruebas en caso de ser necesario.
8. **Validez de los Resultados.** Realidad $\leftrightarrow$ Resultados $\leftrightarrow$ Realidad

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