Capítulo 6

Conclusiones

6.1 Conclusiones referentes a las hipótesis planteadas.

Para la primera hipótesis:

El empleo de técnicas de primeros principios para estimar propiedades catalíticas y de tolerancia a especies contaminantes reduce el tiempo de desarrollo de un catalizador.

Para la segunda hipótesis:

Los resultados de la prueba de voltaje de circuito abierto mostrados en la sección 5.2.9.1 demuestran que a menor tamaño de partícula es mayor la capacidad de disociación de hidrógeno.

Para la tercera hipótesis:

Los resultados expresados como el cambio en la energía de quimisorción descritos por la Tabla VII, más la evidencia experimental mostrada por Raghuveer *et al* [115], nos

ayudan a concluir que el compuesto $Pd_{70}Co_{20}Mo_{10}$ tiene una mayor capacidad de tolerancia al CO.

6.2 Conclusiones generales para el ensamble membrana-electrodos.

- La estimación de propiedades catalíticas y de adsorción de especies contaminantes por técnicas computacionales de primeros principios resulta ser una herramienta práctica que, mediante un adecuado proceso de validación de modelos nos puede reducir el tiempo de desarrollo de un elemento catalizador para cualquier reacción química. Por otra parte, el cálculo de las densidades de estados electrónicos (DOS) antes y después de la reacción de disociación de hidrógeno están acorde con las predicciones del modelo de banda "d" para la reactividad de superficies metálicas.

- La técnica de deposición de nanopartículas por condensación de gas inerte (IGC) es confiable y repetible, además de que es posible tener control muy preciso sobre el tamaño de partículas generadas en condiciones de ultra-alto vacío, y no requiere de la utilización de agentes químicos que contaminen el ambiente. Existe una buena homogeneidad en la distribución de partículas sobre los sustratos con un muy bajo nivel de contaminación por otras especies.

- La técnica de espectroscopia de electrones Auger (AES) resultó de mucha utilidad para obtener el perfil de composición de los depósitos de nanopartículas sobre el sustrato de Si (100). Al ser una técnica de análisis de superficie, el perfil de composición obtenido es referente al nivel superficial de la película depositada, pero una aproximación razonable fue el comparar este perfil con el obtenido para el target original de $Pd_{70}Co_{20}Mo_{10}$.

- La técnica de microscopia de fuerza atómica de contacto nos permitió obtener una imagen de las nanopartículas depositadas sobre el sustrato de Si (100) y sobre la membrana de Nafion 112. A través de esta técnica fue posible estimar el tamaño de los aglomerados formados por las partículas depositadas.

- El análisis de espectroscopia FTIR nos permite identificar la presencia de los elementos del compuesto trimetálico a través de las bandas de absorción de los grupos funcionales presentes en Pd-Co-Mo/Si(100) y Pd-Co-Mo/C/nafion 112, basándonos en la información disponible en la literatura [109, 138-141]. Además, fue posible mediante la identificación de las bandas de absorción correspondiente a cada grupo funcional, localizar las interacciones con carboniles y la formación de un óxido en el caso de Co.

- La caracterización en la celda de combustible tipo PEM nos permite considerar el compuesto trimetálico Pd-Co-Mo con composición química (70:20:10%) como un buen candidato para sustituir al Pt puro como elemento

catalizador tanto en la reacción anódica como en la reacción catódica, considerando una eficiencia del 25 % (para el tamaño de partícula de 3 nm) con respecto a la prueba de voltaje de circuito abierto bajo las condiciones de preparación del ensamble manejadas en este trabajo.

- El costo total de producción de un ensamble MEA desarrollado mediante esta metodología resulta ser menor al de un catalizador de Pt comercial, cuando se considera una superficie de 25 cm^2 por corrida de producción.

6.3 Trabajos futuros.

El presente trabajo permite sentar las bases de mi trabajo futuro, ya que aún existe mucho trabajo por hacer en el área de catalizadores para celdas de combustible.

La optimización del ensamble MEA propuesto en el presente trabajo, la búsqueda de mejores compuestos con una mayor actividad catalítica y más tolerantes a las especies moleculares contaminantes, serán la base de los futuros trabajos de investigación a realizar.

Además, se pretende desarrollar otras líneas de investigación como la aplicación de los materiales nanoestructurados en medicina, semiconductores y otros procesos de catálisis.

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Inglés 100 %

AREAS DE ESPECIALIDAD

Investigación y Desarrollo de materiales nano-estructurados para celdas de combustible, semiconductores y anticorrosivos
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Mantenimiento Proactivo y Análisis de Aceite	(16 horas)
Las Mejores Prácticas de Lubricación	(16 horas)
Termografía Infrarroja	(16 horas)
Desarrollo de Habilidades de Supervisión	(20 horas)
Principios Gerenciales	(40 horas)
Programación de Manipuladores Robóticos	(40 horas)
Controladores Lógicos Programables	(40 horas)
Electricidad y Electrónica Industrial	(40 horas)
Electro-neumática	(16 horas)
Hidráulica	(20 horas)
Drives, Inversores y Servo-mecanismos	(60 horas)
Desarrollo de Instructores Técnicos	(40 horas)
Combate a incendios industriales	(40 horas)
Primeros auxilios	(40 horas)

ARTICULOS CON ARBITRAJE INTERNACIONAL

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CAPITULOS DE LIBROS

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PUBLICACIONES EN CONGRESOS INTERNACIONALES

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Modeling and simulation of CO adsorption by Pt and $Co_{50}Ni_{50}$ catalysts

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Abstract: Purpose of this article is to report results obtained by computer modeling and simulation using ab-initio techniques for CO adsorption on Pt (1 1 0) and $Co_{50}Ni_{50}$ fuel cells catalysts. From these results, comparison has been made to show different CO adsorption strengths. This is the first step to make an efficient engineering that allows us to obtain high-performance, low-cost nanostructured catalysts.

Keywords: Catalyst, fuel cell, nanostructure, ab-initio, CO adsorption, CASTEP

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Comparison of Pt and $Co_{50}Ni_{50}$ composites for sulfur poisoning

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Abstract: Purpose of this article is to report results obtained by computer modeling and simulation using ab-initio techniques for sulfur adsorption on Pt (1 1 0) and $Co_{50}Ni_{50}$ (1 1 0) compounds. From these results, comparison has been made to show different S adsorption strengths considering short bridge and on-top mechanisms.

Keywords: fuel cell, sulfur adsorption, bimetallic compound, ab-initio

Fe-filled carbon nanotubes produced by microwave heating of ferrocene.

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Abstract

Highly efficient one-step microwave technique (MW) was applied to obtain long and aligned carbon nanotubes with or without Fe filling. Carbon nanotubes (CNTs) were produced by microwave irradiation heating from a ferrocene $Fe(C_5H_5)_2$ as a precursor. Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and Atomic Force Microscopy (AFM) were used to study the growth process of aligned carbon nanotubes during microwave heating. Formed CNTs have a metal particle at the tip of each tube. This carbon nanostructure promises attractive for nanoscale engineering of fuel cells and other systems.

Keywords: Carbon nanotubes, microwave irradiation, Fe-particle, Hamada indexes, atomic force microscopy.

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