

Magnetocrystalline Anisotropy as a Design Principle in PtPdFe Intermetallic Alloys for Fuel Cell Electrocatalysis

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Ordered Pt-based intermetallic alloys are emerging as efficient oxygen reduction reaction (ORR) electrocatalysts in hydrogen fuel cells, outperforming their disordered counterparts. However, the intrinsic role of atomic ordering in governing ORR catalytic performance remains unclear. In this work, we report ferromagnetic PtPdFe ternary intermetallics with structurally ordered tetragonal L₁₀ and cubic L₁₂ phases (Figure 1a), each featuring distinct crystal structures and atomic arrangements. Our study highlights magnetocrystalline anisotropy as a key structure-dependent descriptor that governs ORR activity in these alloys. Electrochemical half- and single-cell tests reveal that L₁₀-PtPdFe magnetic intermetallic catalysts (MICs) deliver higher ORR activity than their L₁₂ counterparts (Figure 1b). Combined experimental and theoretical analyses attribute this enhancement to the unique tetragonal L₁₀ structure, where strong 5d–3d orbital interactions along the c-axis induce ferromagnetic ordering and elevate magnetocrystalline anisotropy energy, thereby accelerating ORR kinetics. Furthermore, membrane electrode assemblies fabricated by L₁₀-PtPdFe cathode MICs sustain fuel cell performance beyond the 2025 US Department of Energy stability targets under H₂–O₂, H₂–air, and H₂–N₂ conditions. These findings establish a new design principle for Pt-based intermetallic catalysts, demonstrating that magnetic anisotropy arising from ferromagnetic ordering can be strategically harnessed to optimize fuel cell performance.

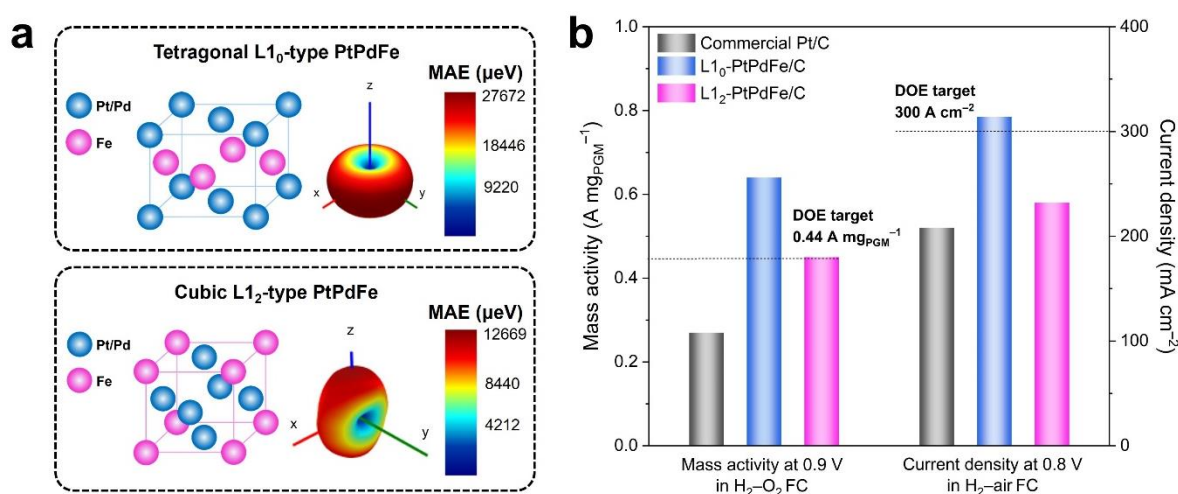


Figure 1. (a) Crystal structures of L₁₀- and L₁₂-type PtPdFe and their magnetocrystalline anisotropy energy (MAE) values. (b) Mass activity at 0.9 V and current density at 0.8 V of commercial Pt/C, L₁₀-PtPdFe/C, and L₁₂-PtPdFe/C catalysts under H₂–O₂ and H₂–air fuel cells, respectively.

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Supplementary Pages

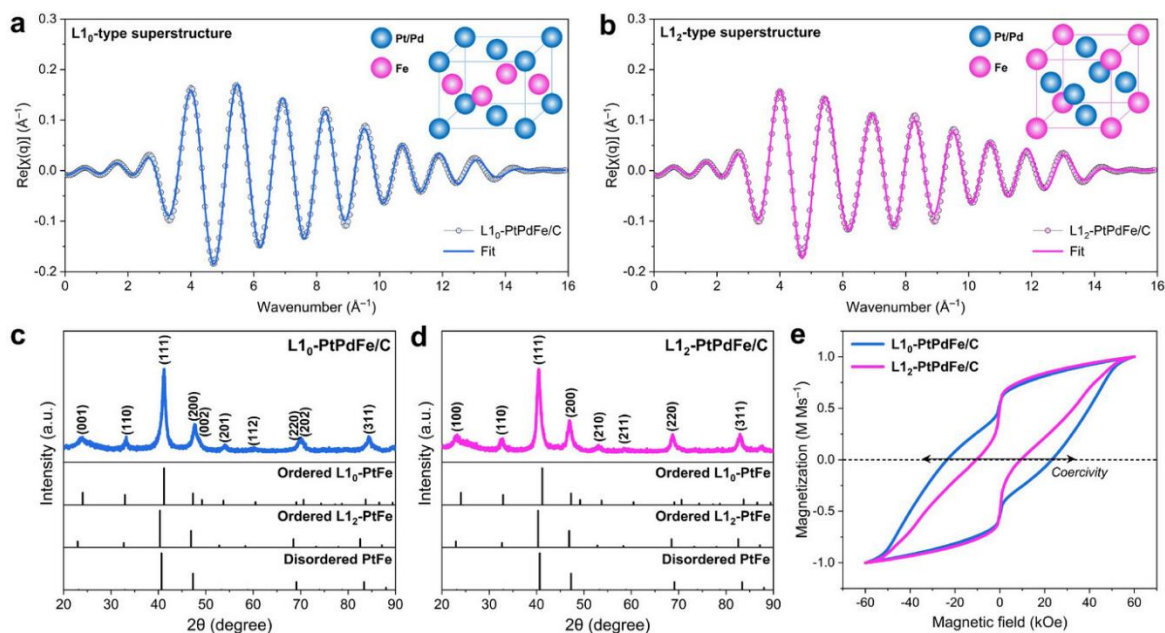


Figure 2. The k -weighted EXAFS oscillations in q -space of a) L1₀-PtPdFe/C and b) L1₂-PtPdFe/C for L1₀- and L1₂-type superstructure fittings, respectively. XRD patterns of c) L1₀-PtPdFe/C and d) L1₂-PtPdFe MICs. The peaks are indexed by disordered cubic A1-PtFe (PDF #03-065-9122), ordered tetragonal L1₀-PtFe (PDF #03-065-9121), and ordered cubic L1₂-PtFe (PDF #01-089-2050). e) Room-temperature magnetic hysteresis (M–H) loops of L1₀-PtPdFe/C and L1₂-PtPdFe/C MICs.