Electronic Supplementary Information

Thermally stable and coke resistant CoMo alloy-based catalysts as fuel electrodes for solid oxide electrochemical cells

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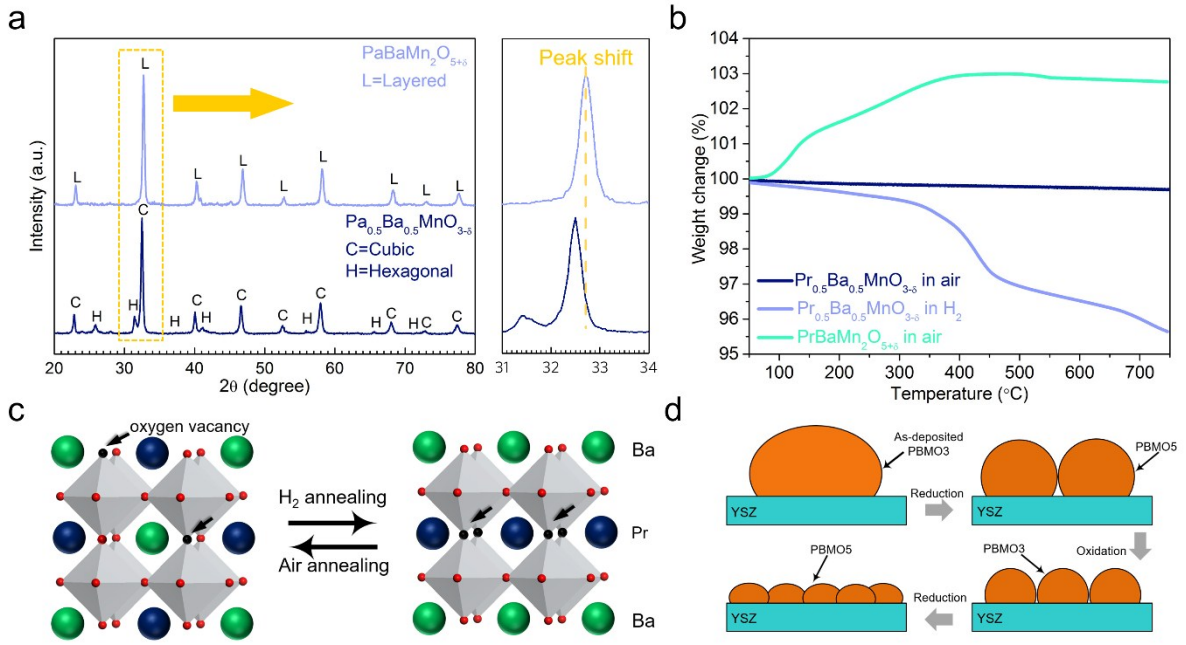

Figure S1. (a) XRD profiles of the PBMO3 and PBMO5 powders; (b) TGA tests of PBMO3 and PBMO5 powders in various atmospheres. (c) crystal structure transformations of PBMO3 and PBMO5 upon reduction and oxidation; (d) redox process induced mosaic-like YSZ@PBMO5 scaffold.

The X-ray diffraction pattern has revealed that the as-deposited PBMO3 is a mixture of cubic structure PBMO3 and hexagonal structure $BaMnO_3$. Upon reduction, it displayed remarkable loss of oxygen (Thermal Gravity Analysis, TGA in Figure S1b), resulting in a phase change that is associated [1, 2].

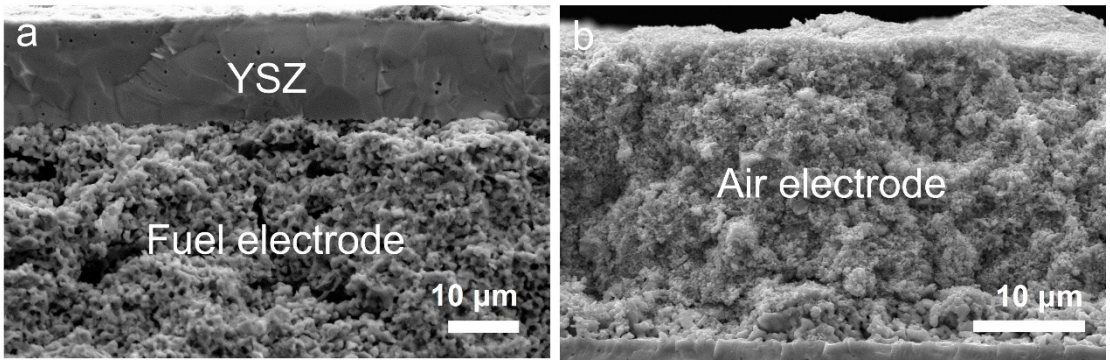

Figure S2. (a) and (b) SEM images of the cell components.

The microstructures of other cell components were examined by scanning electron microscopic (SEM), as illustrated in Figure S2. The cell substrate was composed of a ~10 μm dense YSZ layer and a ~1 mm porous YSZ layer, which was fabricated through classical tape casting and co-sintering processes (Figure S2a). After calcination at 1400 °C, the thin YSZ layer was fully densified, and no obvious pores were observed, ensuring the gas tightness. The porous YSZ functioned as the fuel electrode support to carry the infiltrated oxides and metallic. The porosities of the support measured by the Archimedes method were 54% after fabrication and 43% after infiltrations, respectively. Such a high porosity could effectively eliminate the mass-transport limitations raised due to slow gas diffusion. An NBCaCF-GDC ($NdBa_{0.75}Ca_{0.25}Co_{0.85}Fe_{0.15}O_{3-\delta}$-$Gd_{0.1}Ce_{0.9}O_{1.9}$) composite was fabricated on top of the electrolyte to serve as the air electrode, which exhibited good adhesion to the electrolyte and had a homogenous 3D porous structure with a thickness of 30 μm (Figure S2b).

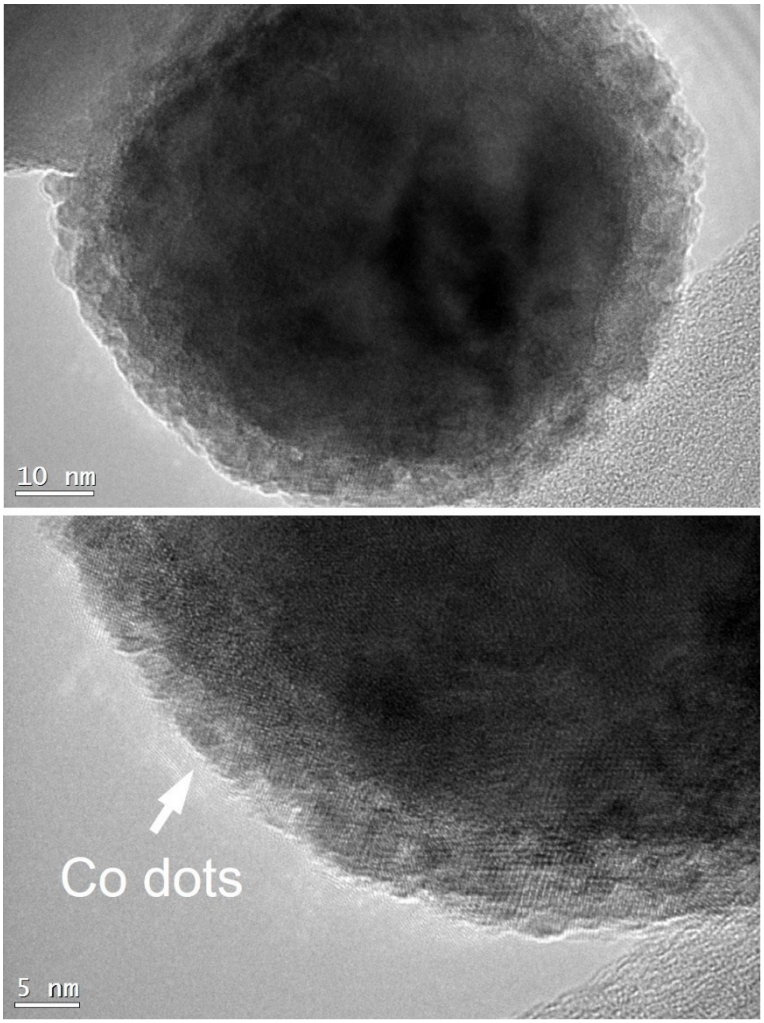

Figure 3. HRTEM image of a CoMo nanoparticle, showing the crystalline Co shell. The Co shell consists of a number of Co minicrystals, denoted as Co dots.

Many minicrystals have been found on the surface of the CoMo NAs.

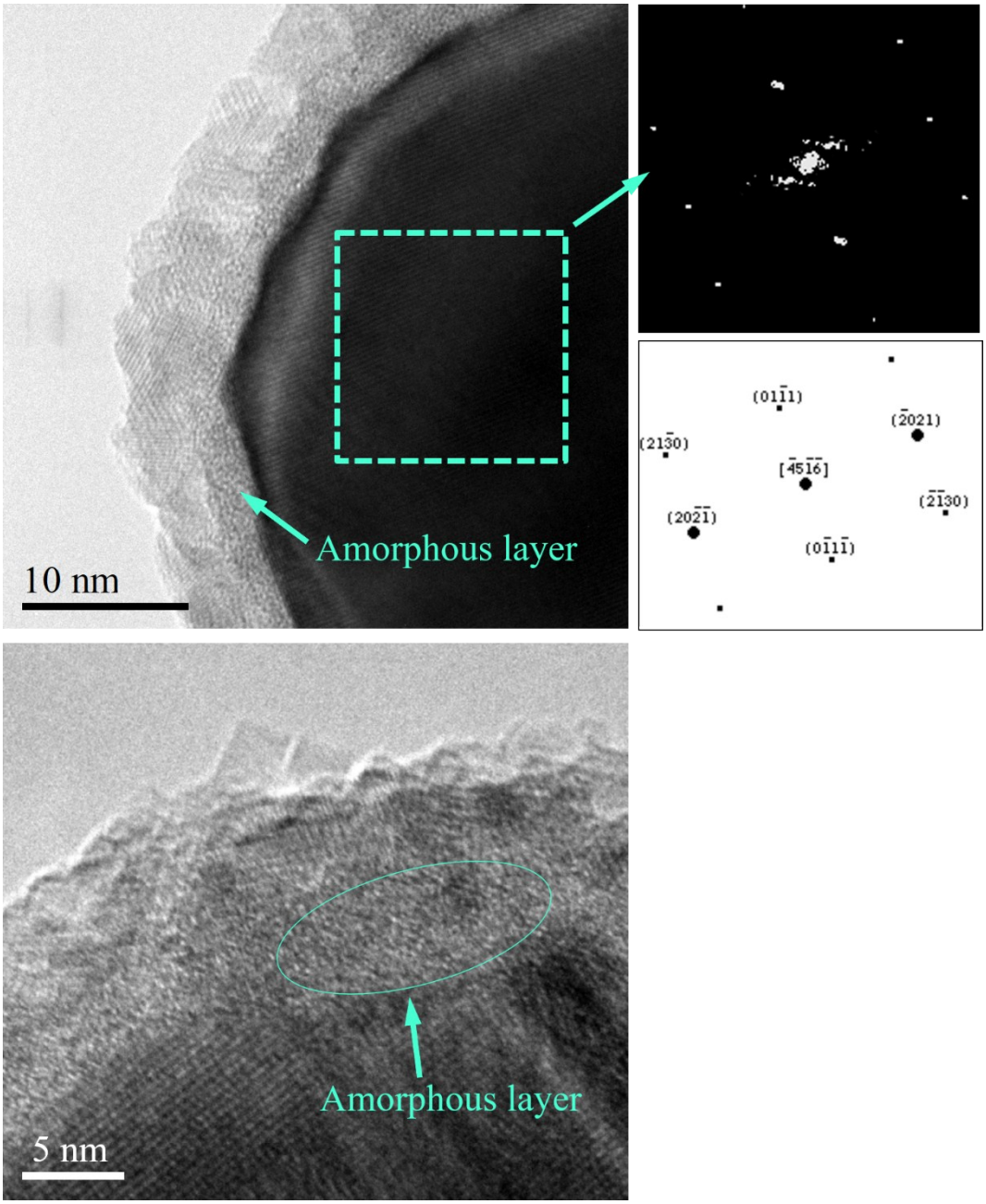

Figure S4. HRTEM image of a CoMo nanoparticle, and the corresponding SAED and simulation.

The results confirm that the core is the hexagonal structure Co_3Mo that belongs to the space group: P63/mmc (194). The measured cell parameters are a=b=0.513 nm, c=0.412 nm, α=β=90 °, γ=120 °.

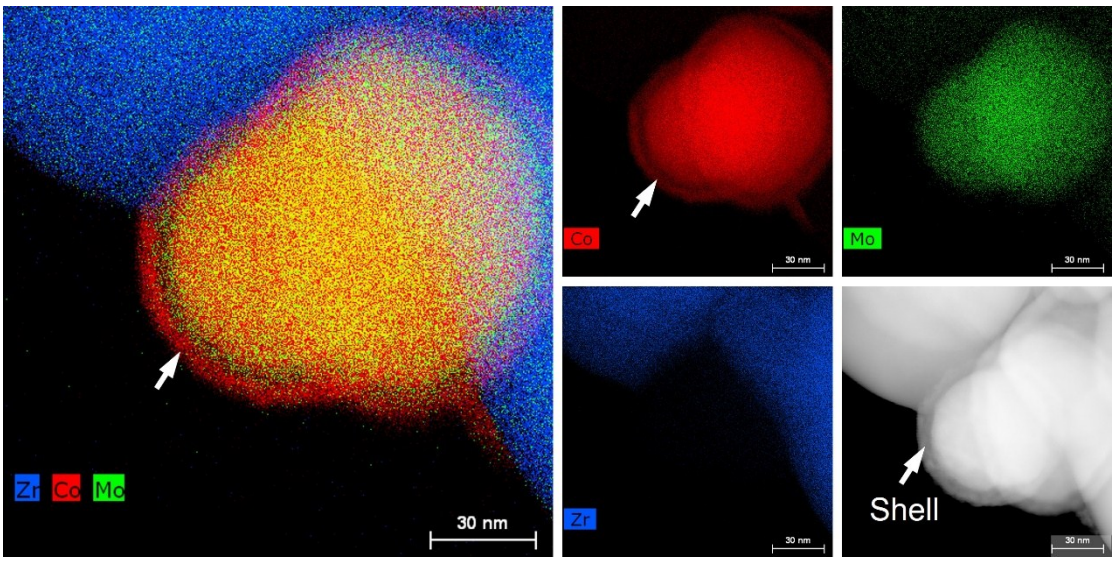

Figure S5. HAADF-EDX results of the CoMo sample, showing the Co shell, amorphous Mo sub-shell and Co_3Mo core.

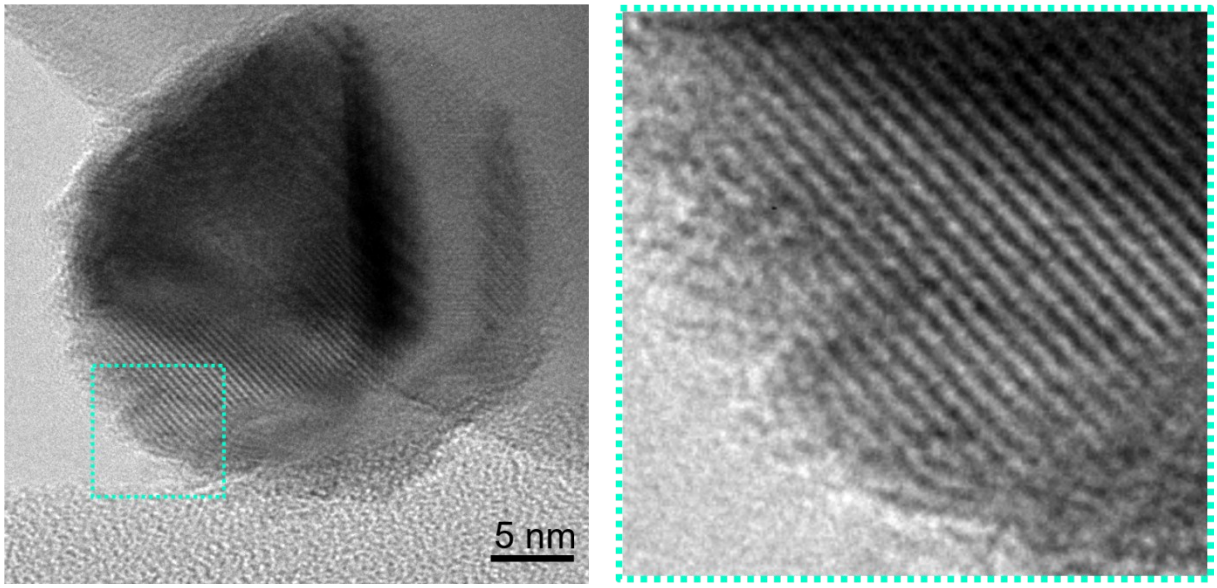

Figure S6. HRTEM image of a Co nanoparticle, showing that no double shell structure has been observed.

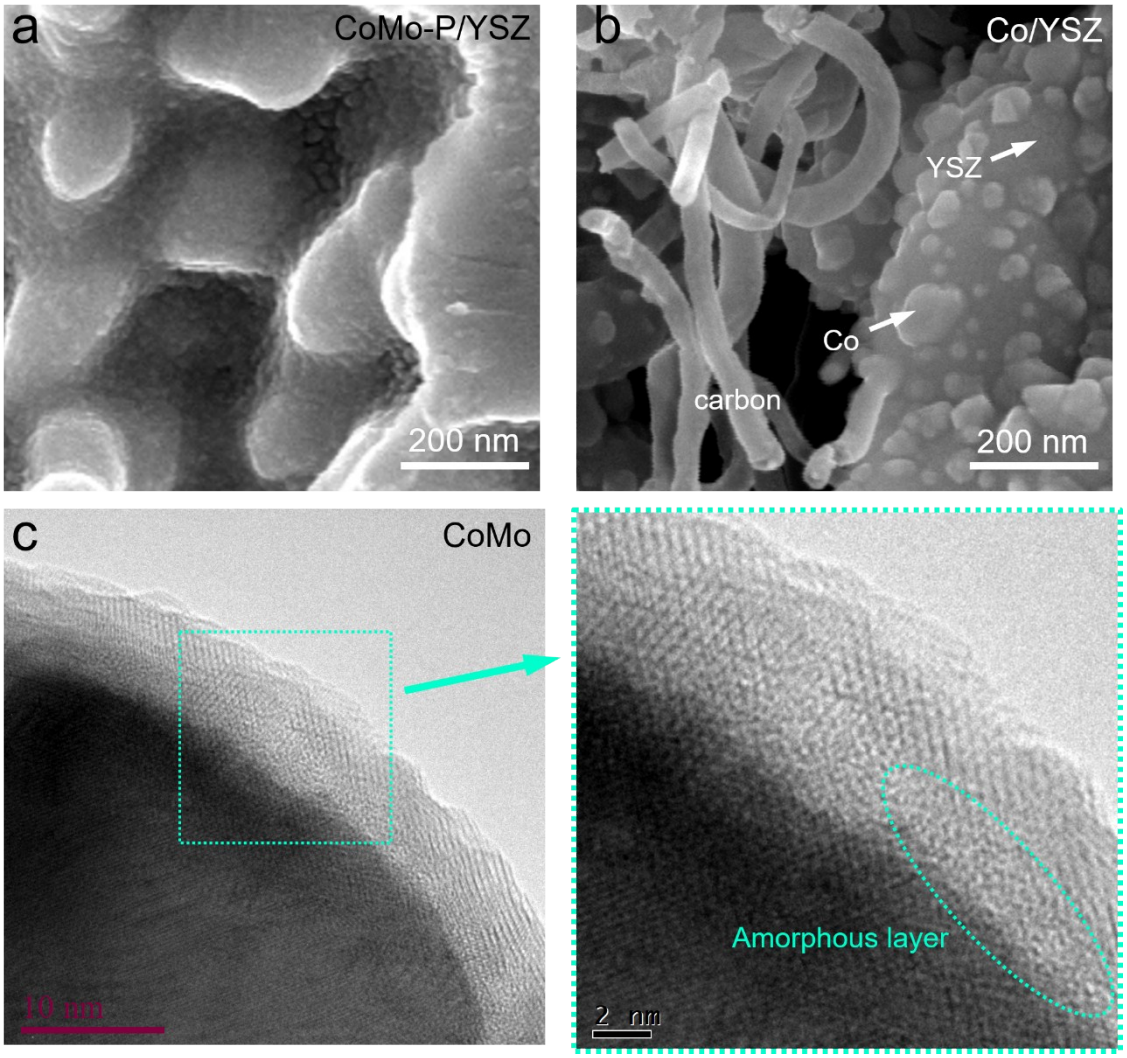

Figure S7. The SEM images of CoMo-P/YSZ (a) and Co/YSZ (b) cells after the stability tested shown in Figure 4b; (c) HRTEM image of a CoMo nanoparticle after the stability test shown in Figure 5b.

Reference

1. S. Sengodan, S. Choi, A. Jun, T. H. Shin, Y. W. Ju, H. Y. Jeong, J. Shin, J. T. Irvine, G. Kim, Nat. Mater. 14 (2015) 205-209.
2. O. Kwon, S. Sengodan, K. Kim, G. Kim, H. Y. Jeong, J. Shin, Y.-W. Ju, J. W. Han, G. Kim, Nat. Commun. 8 (2017) 15967.