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Figure A1 Effect of time on stream on the stability of 7CuO/CeO₂ under PROX reaction.



Figure A2 CO conversion of 1Au/CeO₂ for PROX reaction using feed composition of 1%CO, 1%O₂, 40%H₂ balance in He.



Figure A3 Selectivity of $1Au/CeO_2$ for PROX reaction using feed composition of 1%CO, $1\%O_2$, $40\%H_2$ balance in He.



Figure A4 CO conversion of 1Au/CeO₂ with different step of DP method for PROX reaction.



Figure A5 CO conversion of 7CuO/CeO₂ with different step of DP method for PROX reaction.



Figure A6 CO conversion of pure MSP ceria for PROX reaction using feed composition of 1%CO, 1%O₂, 40%H₂ balance in He.

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Figure A7 Selectivity of pure MSP ceria for PROX reaction using feed composition of 1%CO, 1%O₂, 40%H₂ balance in He.

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Calculation A1 Scherrer's equation.

$$L = \frac{K\lambda}{\beta . \cos\theta}$$

where L = the average crystallite size

- λ = the X-ray wavelength in nanometer (nm)
- β = the peak width of the diffraction peak profile at half maximum height in radians
- K = constant related to crystallite shape; spherical crystals with cubic symmetry is 0.94
- θ = the diffraction peak position

<u>Example</u>: Calculate the average crystallite size of pure MSP ceria from the diffraction peak at $2\theta = 28.5479^\circ$, $\beta = 2.2819^\circ$ by using the X-ray wavelength at 0.15406 nm

First: Convert β from degrees to radians

 $\beta = 0.0398$ radians

Second: Calculate $\cos\theta$ from the diffraction peak at $2\theta = 28.5479^{\circ}$ (the θ can be in degrees or radians, since the $\cos\theta$ corresponds to the same number)

Final: Using above equation to determine the average crystallite size

 $L = \frac{0.94 \times 0.15406 nm}{0.0398 radius \times \cos(14.2740^\circ)} = 3.750 nm$

Calculation A2 Lattice parameter by considering as a cubic crystal.

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

where d = d-spacing

$$h,k,l = plane(h,k,l)$$

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a = cell parameter

Example: Calculate the lattice parameter from a plane (1,1,1) which has a spacing between this plane of 3.1244 $\stackrel{o}{A}$

$$\frac{1}{3.1244^2} = \frac{1^2 + 1^2 + 1^2}{a^2}$$
$$a = 5.4116 \quad \stackrel{o}{A}$$

Calculation A3 calculation of the amount of Ce^{3+} (%) on the surfaces of ceria based catalysts.

$$Ce^{3+}(\%) = \frac{S(Ce^{3+})}{S(Ce^{3+} + Ce^{4+})} \times 100$$

where $S(Ce^{3+}) = v^{0} + u^{0} + v' + u'$

0

$$S(Ce^{4+}) = v + u + v' + u' + v'' + u''$$

Example: Calculate the amount of Ce^{3+} (%) on the surfaces of pure MSP ceria

$$S(Ce^{3+}) = 5.4 + 10.3 + 11.3 + 15.7 = 42.7$$

$$S(Ce^{4+}) = 9.2+5.4+10.3+18.4+11.3+15.7 = 70.3$$

$$Ce^{3+}(\%) = \frac{42.7}{70.3 + 42.7} \times 100 = 37.8$$

Calculation A4 Kubelka-Munk function.

$$f(r) = \frac{(1-r)^2}{2r}$$

where f(r) = Kubelka-Munk function

r = reflectance fraction

Example: Convert the reflectance(%) of 47.0 (at the wavelength of 200 nm) to the absorbance

First: Convert reflectance(%) into fraction

reflectance(fraction) =
$$\frac{47.0}{100} = 0.47$$

Second: Convert the reflectance into absorbance

$$f(r) = \frac{(1 - 0.47)^2}{2 \times 0.47} = 0.30$$

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