Physical modeling of catalyst degradation in low temperature fuel cells: platinum oxidation, dissolution, particle growth and platinum band formation - Supplementary material

Thomas Jahnke[1,*], Georg A. Futter[1], Andrea Baricci[2], Claudio Rabissi[2], and Andrea Casalegno[2]

[1]German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Computational Electrochemistry, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany
[2]Politecnico di Milano, Dipartimento di Energia via Lambruschini 4, 20156 Milano, Italy
[*]Corresponding author. thomas.jahnke@dlr.de

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In the following we calculate the fraction of edge sites for the truncated octahedron and compare it to the relation for the cuboctahedron derived by Redmond et al. [1].

The truncated octahedron consists of 14 faces, 36 edges and 24 vertices. If l is the length of the edges then the number of atoms along each edge is given by

$$n = \frac{l}{2.77\text{Å}}, \tag{1}$$

with 2.77Å being the distance between the platinum atoms. By setting the volume of the truncated octahedron $V = 8\sqrt{2}l^3$ equal to the volume of a corresponding spherical particle, we obtain a relation between number of atoms along one edge and the particle radius

$$n = \left(\frac{\pi}{6\sqrt{2}}\right)^{1/3} \frac{r}{2.77 \cdot 10^{-10}\text{m}}, \tag{2}$$

The total number of edge and kink atoms is given by $36(n-2)+24$, the number of atoms on the six square faces is $6(n-2)^2$ and the number of atoms on the eight hexagonal faces is $8(3n^2-9n+7)$. Thus, the fraction of edge sites for the

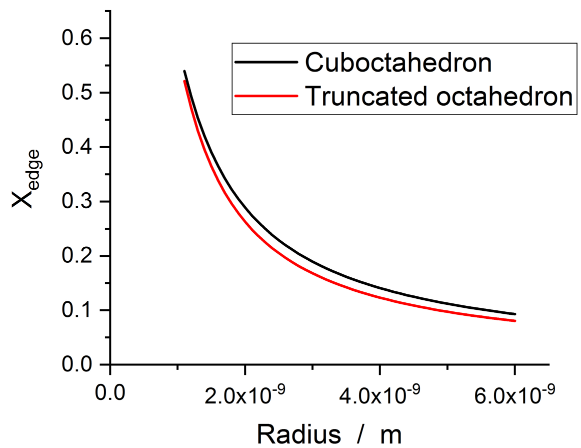

Figure 1: Fraction of edge sites for cuboctahedron (black) and truncated octrahedron (red) particle geometries.

truncated octahedron is given by

$$X_{\text{edge},1} = \frac{36(n-2)+24}{30n^2-60n+32}, \tag{3}$$

For the cuboctahedron Redmond et al. [1] obtained

$$X_{\text{edge},2} = \frac{12+24(n_2-2)}{6(n_2-2)^2+4(n_2-3)(n_2-2)+12+24(n_2-2)}, \tag{4}$$

with the number of atoms along the edge given by

$$n_2 = \left[\frac{4\pi}{\sqrt{50}}\right]^{1/3} \frac{r}{2.77 \cdot 10^{-10}\text{m}}, \tag{5}$$

Fig. 1 shows the comparison between both geometries. As one can see, the dependence of X_{edge} on the particle radius is very similar.

References

[1] E. L. Redmond, B. P. Setzler, F. M. Alamgir, T. F. Fuller, Elucidating the oxide growth mechanism on platinum at the cathode in PEM fuel cells, Physical Chemistry Chemical Physics 16 (11) (2014) 5301. doi:10.1039/c3cp54740j.