Structure Model of Bimetallic PtRu Nano-catalysts by X-ray Absorption Spectroscopy

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Bimetallic nanoparticles (NPs) are of great interest from both a scientific and a technological perspective because the addition of the second metal provides a method to control chemical and physical properties. Bimetallic NPs have been widely exploited for use in catalysis, optoelectronics, information storage, biological labeling. In recent years, XAS studies have been well explored on bimetallic nanoparticles and it shows that the XAS studies focusing on estimation of atomic distributions or alloying extent in the NPs are limited. In our previous work, we have shown that the extent of alloying or atomic dispersion in bimetallic nanoparticles can be determined quantitatively from the structural parameters J_A and J_B of A-B bimetallic NPs derived from XAS From the extent of atomic dispersion or alloying, it is possible to understand and control the structure of bimetallic nanoparticles. Herein, the atomic distributions and extents of alloying of the bimetallic PtRu nanoparticles are studied based of the general XAS methodology. In this work, the synthesis of the bimetallic PtRu colloids was carried out in ethylene glycol solutions containing different concentrations of sodium hydroxide and using different heating methods, as shown in table 1. We have employed the derived expressions for J_A and J_B from the coordination numbers of bimetallic NPs and compared in Table 2. From the quantitative extent of alloying values, we can see that in all the catalysts a considerable amount of Pt is segregated in the core, but the extent of segregation of Pt is higher in PtRuD when compared to the JM 30. The increased value of J_B in the PtRuD catalyst indicated that most of the Ru is involved in alloying and, hence, less segregation of Ru in the shell, whereas in the case of E-TEK 30 catalyst, a lesser extent of Ru is involved in the alloying and considerable extent of segregation of Ru can be expected in the shell region.

Table 1. Sample condition lists

Sample	Method
PtRuA	PtRu/Carbon in EG System without control pH value by Microwave (Pt/Ru (atom%)=1) (acid pH=0.8)
PtRuB	PtRuTi/Carbon in EG System without control pH value by Microwave (Pt:Ru:Ti=1:1:3) (acid pH=0.8)
PtRuC	PtRu/Carbon in EG System without control pH value by heating at 160℃ (Pt/Ru (atom%)=1) (acid pH=0.8)
PtRuD	PtRu/Carbon in EG System control pH value by heating at 160℃ (Pt/Ru (atom %)=1) (base pH=9.45)
JM 30 PtRu/C	(Pt/Ru (atom%)=1) commercial powder
ETEK 30 PtRu/C	(Pt/Ru (atom%)=1) commercial powder

Table 2. Structural coordination number parameters and alloying extent

Sample	A	B	P	R	J_A	J_B
JM 30	8.26	7.09	0.20	0.43	40	86
ETEK 30	8.43	6.72	0.14	0.33	28	66
PtRuA	8.53	6.86	0.11	0.35	22	70
PtRuB	9.23	6.81	0.14	0.35	28	70
PtRuD	9.21	7.06	0.08	0.50	16	100