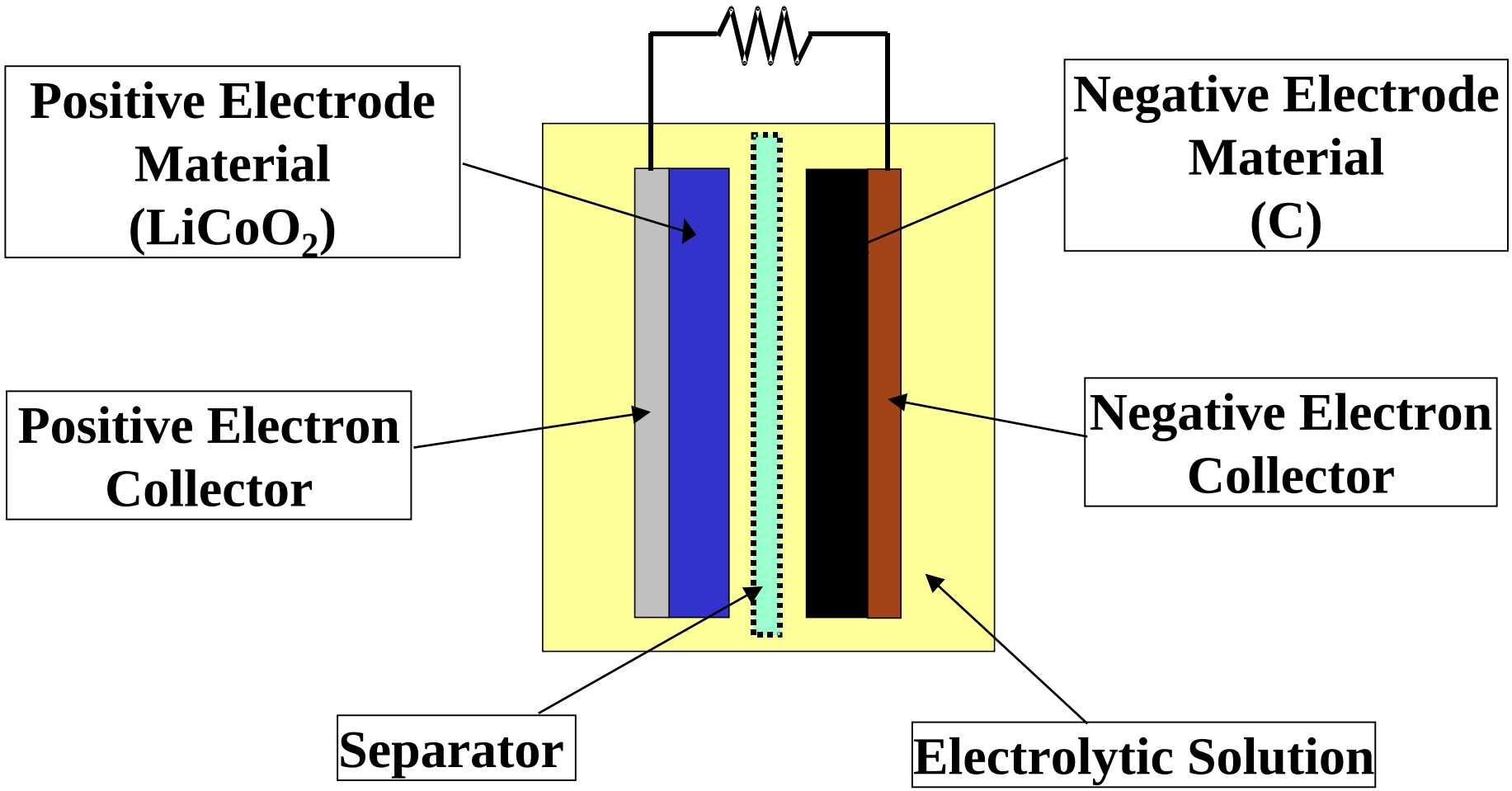
Structural Analysis of Materials for Secondary Battery and Fuel Cell

SANYO Electric Co., Ltd.

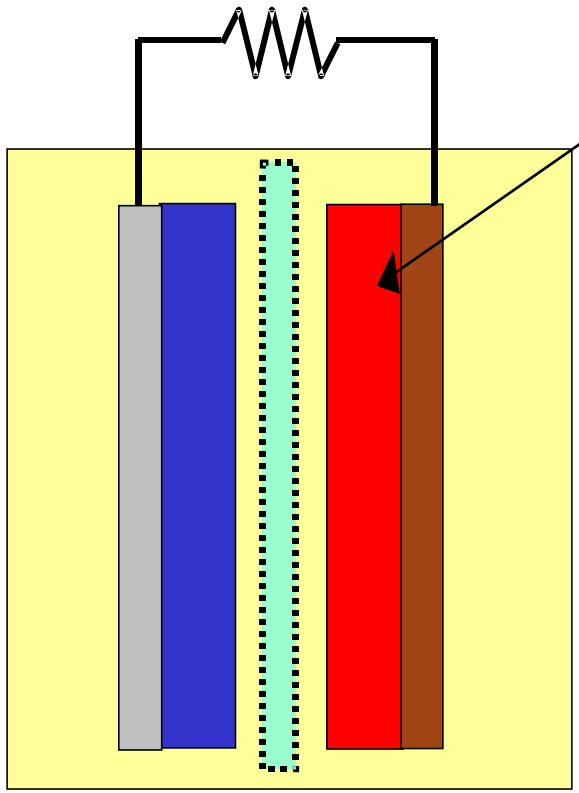
Materials and Devices Development Center BU

Akira MIKAMI

Structure of Lithium Secondary Battery (1)



Structure of Lithium Secondary Battery (2)



Sn Based Negative Electrode Material

1. **Three times larger theoretical capacity compared with C based material.**
2. **High cost performance due to fabrication by electrodeposition.**
3. **Poor capacity performance compared with C based material.**

Samples and XAFS Measurement Conditions

Sample:

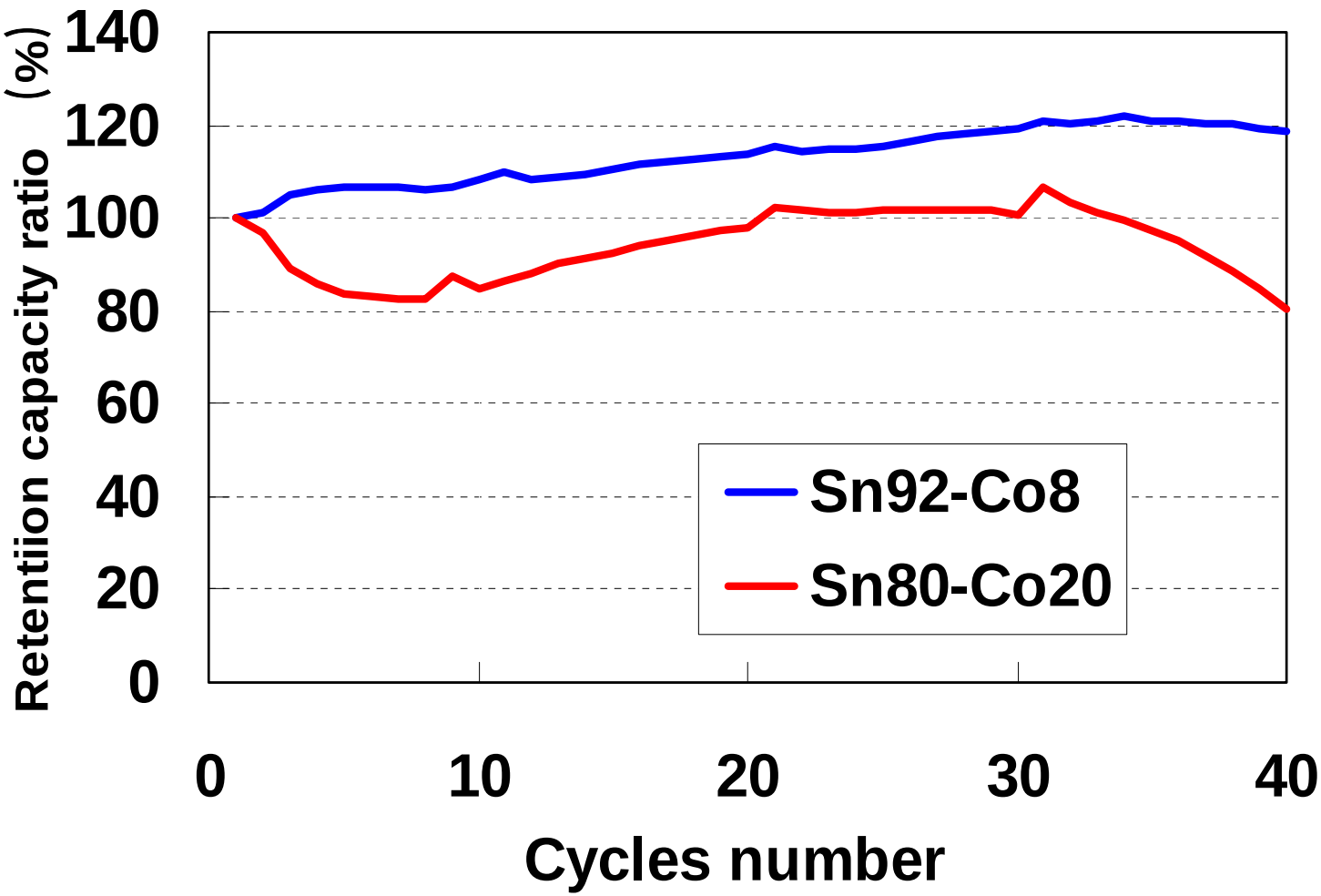
1. Sn80-Co20 Sn:80 wt.% + Co:20 wt.%
2. Sn92-Co8 Sn:92 wt.% + Co:8 wt.%

(before and after charge-discharge cycles)

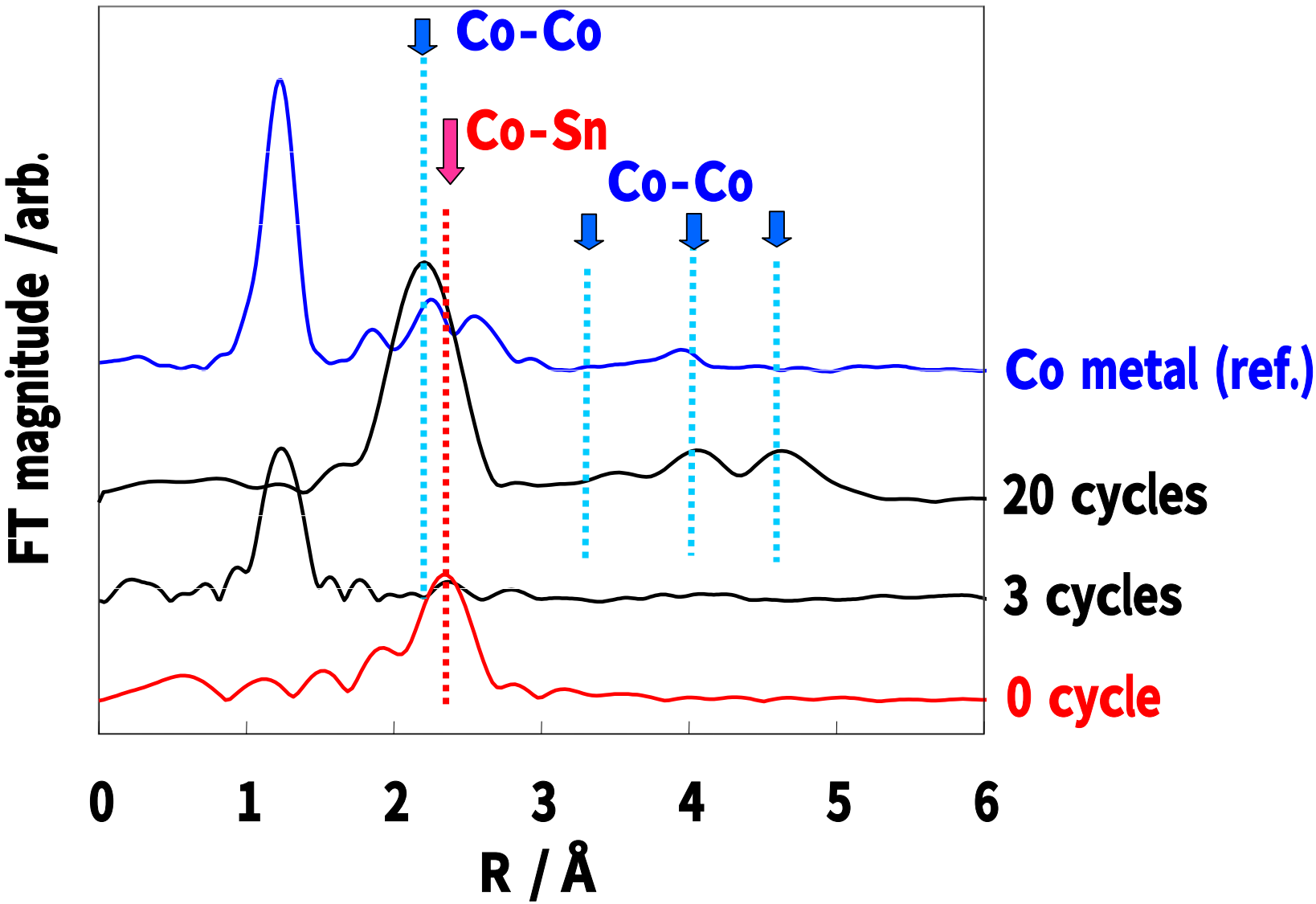
XAFS Measurement Conditions:

1. Fluorescent mode
2. Co K-edge (7.4～9.1keV)
3. Samples are sealed in polyethylene bag

Capacity Performance



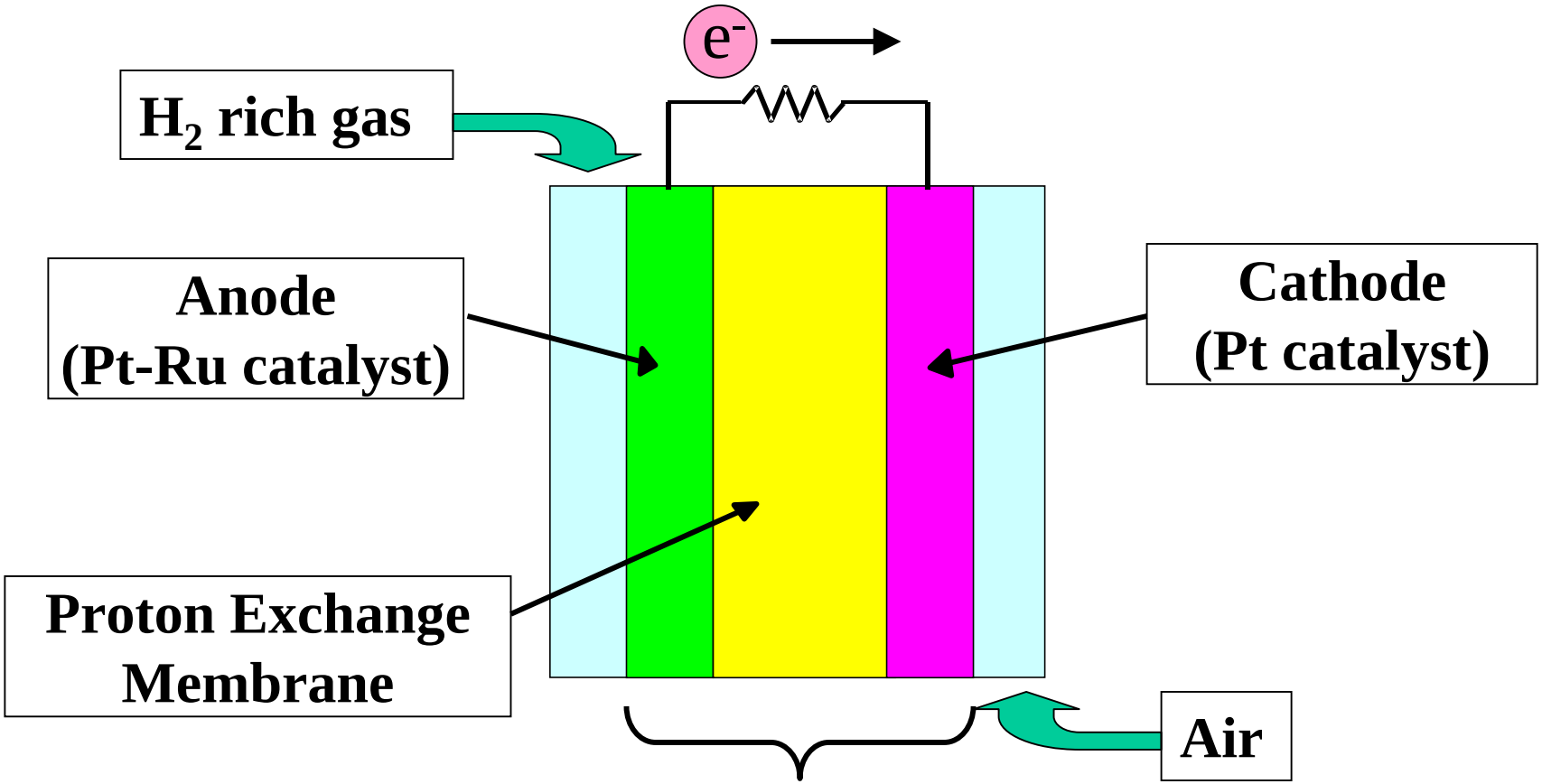
RDF of Sn80-Co20



Conclusions

1. **Structural transformation due to charge-discharge cycles was observed in the case of Sn80-Co20.**
2. **Structural transformation due to charge-discharge cycles was not observed in the case of Sn92-Co8.**
3. **Capacity performance of Sn92-Co8 is better than that of Sn80-Co20. Capacity performance is influenced by structural stability observed by XAFS.**

Structure of PEFC Single Cell



Membrane and Electrode Assembly (MEA)

Samples and XAFS Measurement Conditions

Sample:

Anode and Cathode side of MEA

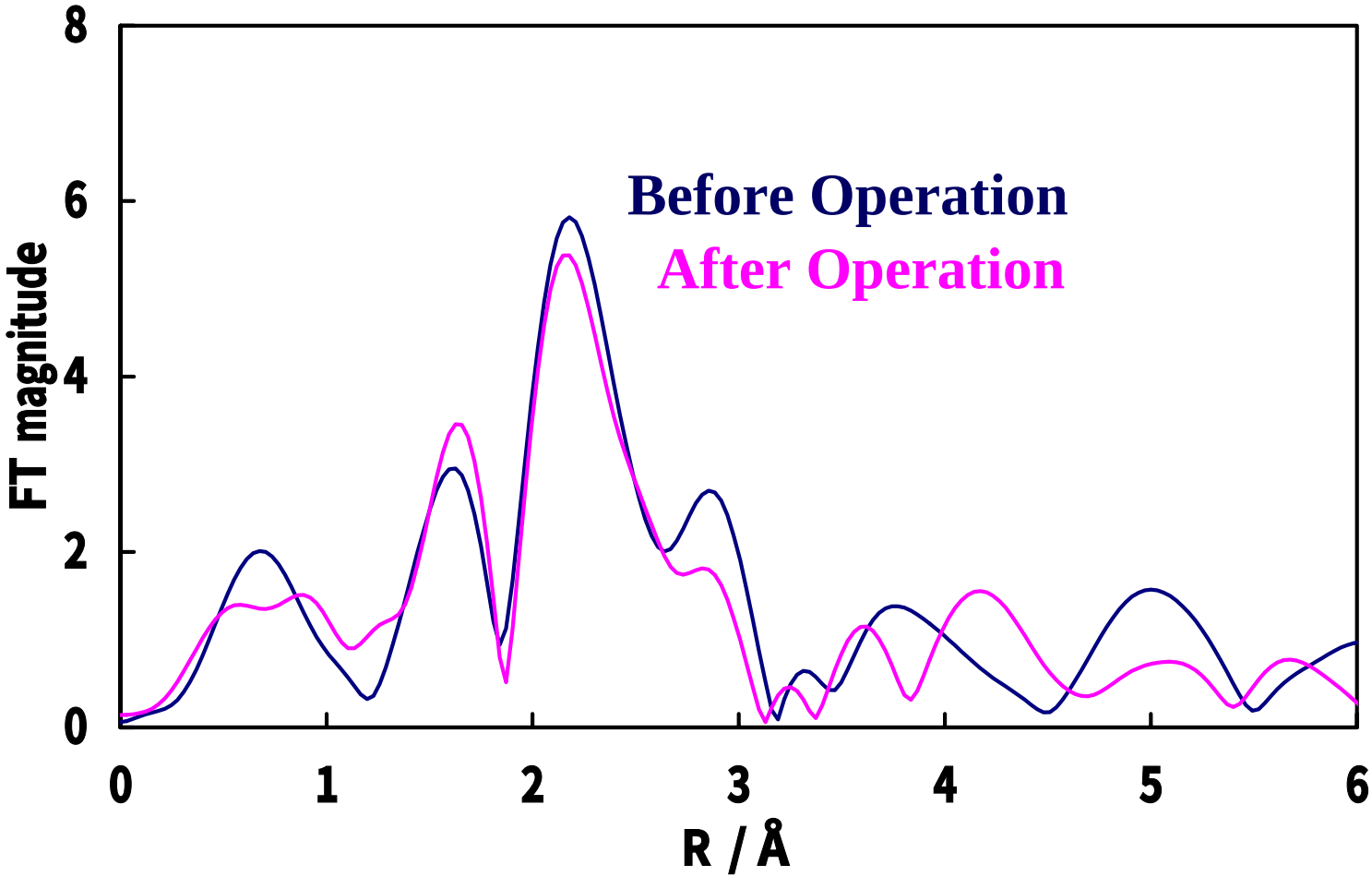
1. **Before operation**
2. **After 3000 hours operation**

XAFS Measurement Conditions:

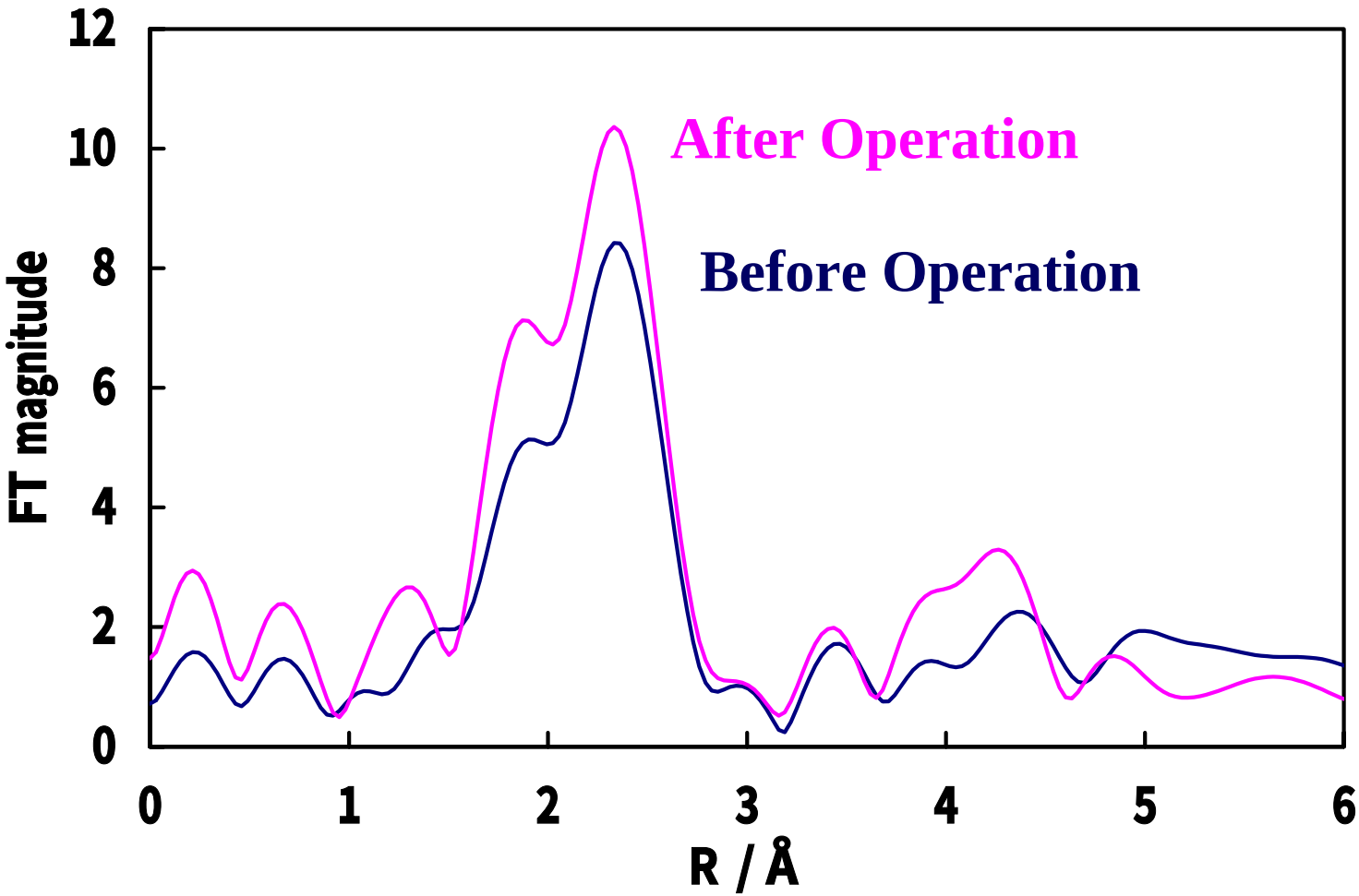
Conversion Electron Yield (CEY) Mode for

1. **Pt L_{III}-edge of both anode Pt-Ru and cathode Pt catalysts**
2. **Ru K-edge of anode Pt-Ru catalysts**

Measured RDF of Pt L_{III}-edge (Anode)



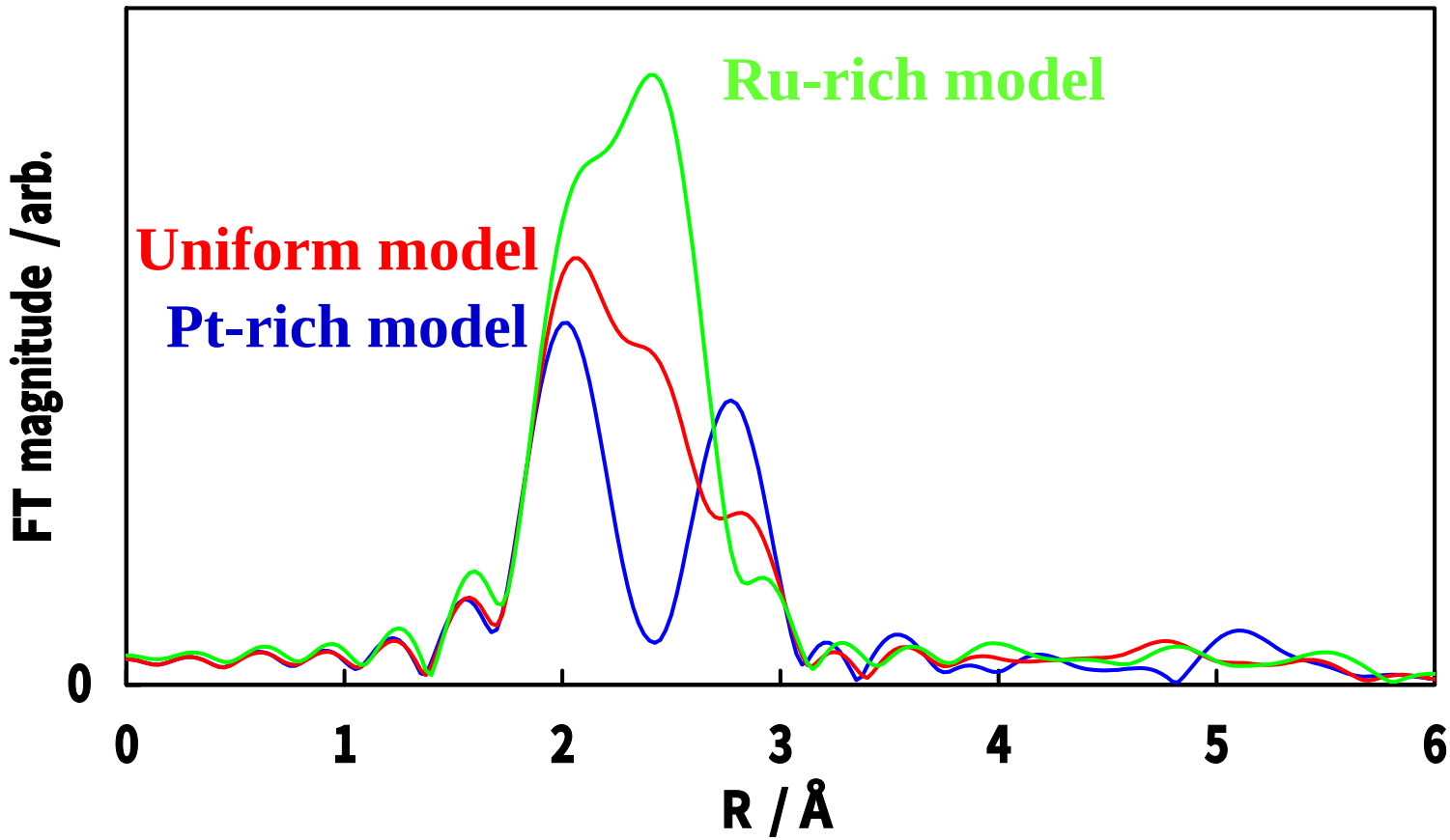
Measured RDF of Ru K-edge (Anode)



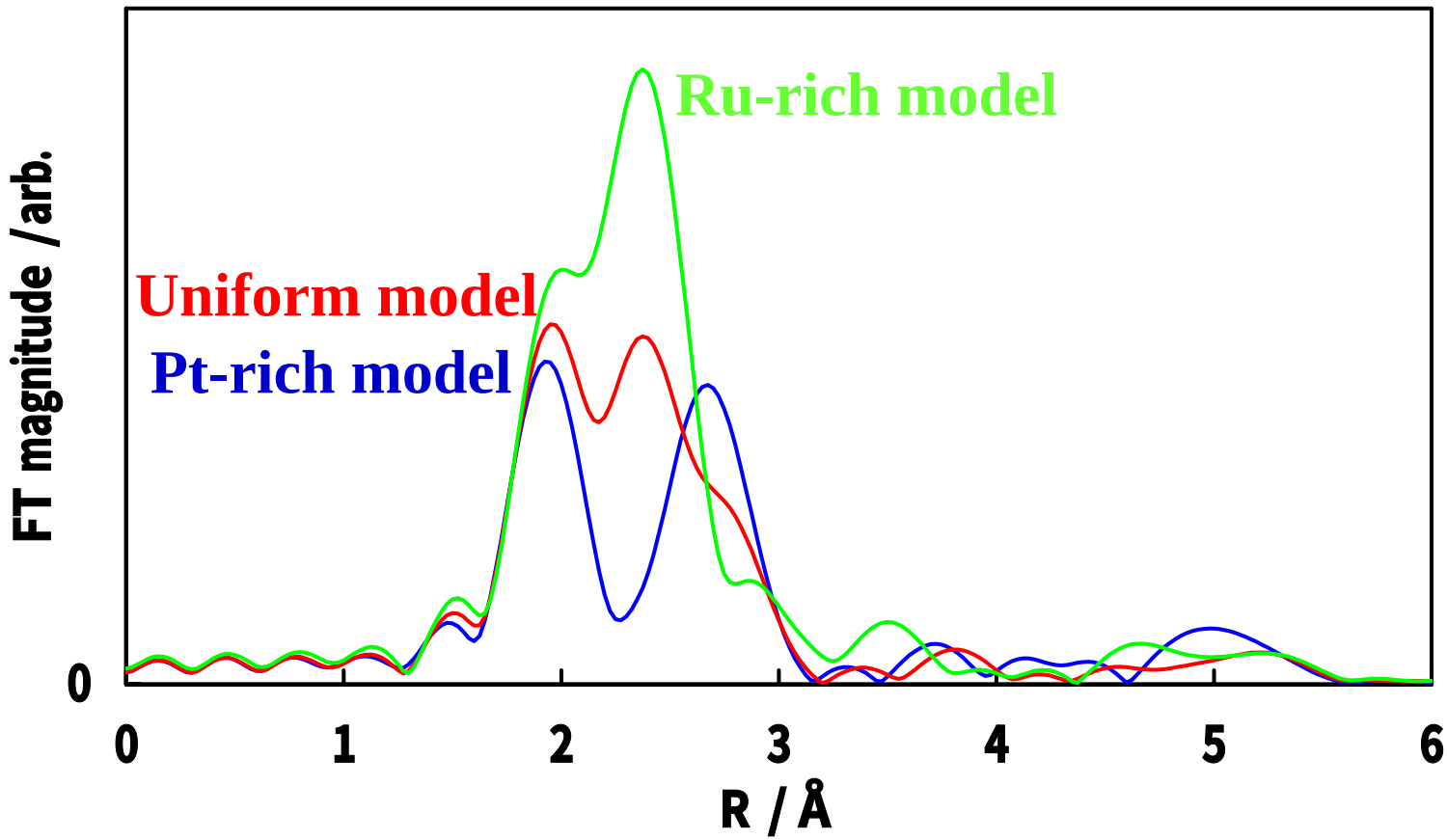
Conditions for FEFF Simulation

1. Assuming fcc like structure (coordination number = 12)
2. Calculations for 3 compositions
   - Pt-rich model Pt:Ru=8:4
   - Uniform model Pt:Ru=6:6
   - Ru-rich model Pt:Ru=4:8
3. Fixing radial distance to the neighbor atom
   - $R_{Ru\text{-}Ru}$ = 2.66 Å
   - $R_{Ru\text{-}Pt}$ = 2.69 Å
   - $R_{Pt\text{-}Pt}$ = 2.71 Å

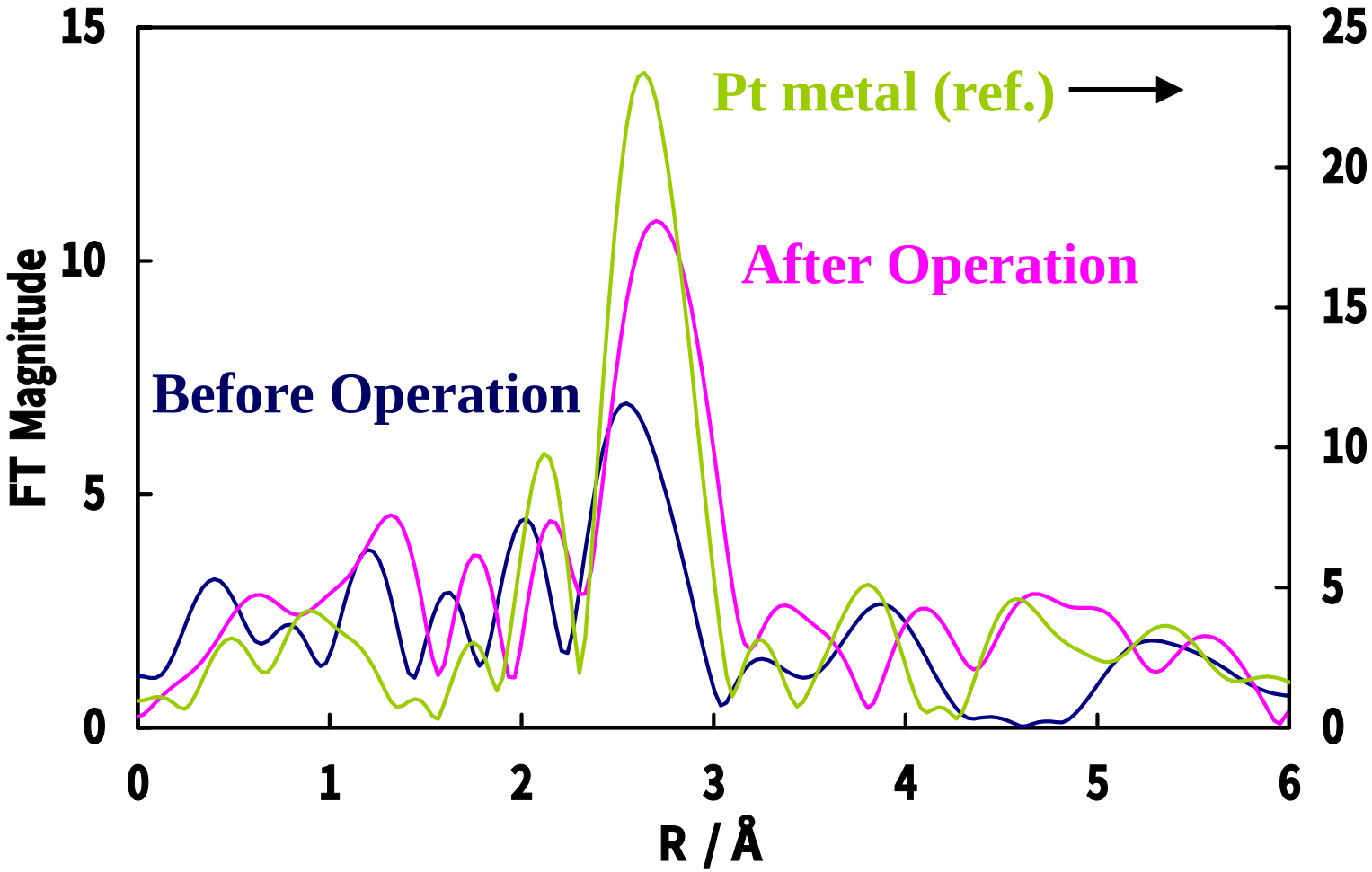
Simulated RDF of Pt L_{III}-edge (Anode)



Simulated RDF of Ru K-edge (Anode)



Measured RDF of Pt L_{III}-edge (Cathode)



Conclusions

1. **The measured RDFs of Pt L_{III}-edge matched the simulation for the Pt-rich model and the measured RDFs of Ru K-edge matched the simulation for the Ru-rich model. Pt and Ru did not distribute uniformly.**

2. **The peak heights of Ru K-edge of anode and Pt L_{III}-edge of cathode after the operation were higher than those before the operation. The particle size might increase during the operation.**