IRCSEM

INOUE LAB.

[Gas levitation furnace and glass]

International Research Center for Sustainable Energy and Materials

http://www.vitreous.iis.u-Tokyo.ac.jp/

Amorphous Materials Design

Department of Materials Engineering

Material Design of Amorphous and Liquid States

We study the materials from an amorphous state to a liquid state. Atomic and electronic structures of the amorphous and liquid states have not been well understood. We study the method in order to understand these materials, and apply it to a variety of materials. Moreover we will produce novel materials and their applications.

♦ Computer Simulations of Amorphous and liquid States

- Total correlation functions
- Molecular dynamics simulations

Novel Titanium/Manganese Redox flow battery

Ti(III)/Ti(V) Mn(II)/Mn(III)

Charge:←, Discharge:→

Anorde

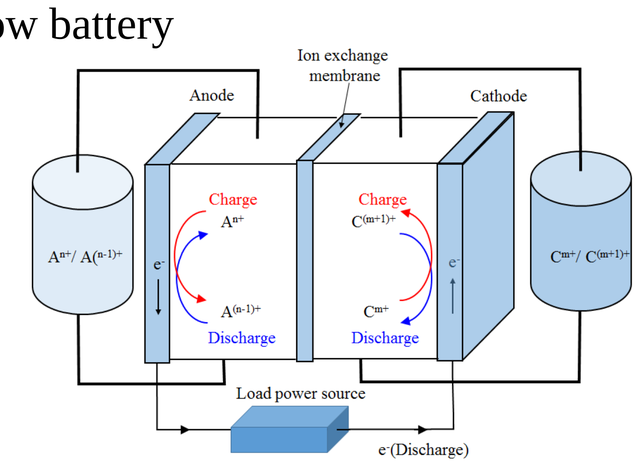
$Ti^{3+} + H_2O \rightleftarrows TiO^{2+} + 2H^+ + e^-$

Cathode

$Mn^{3+} + e^- \rightleftarrows Mn^{2+}$

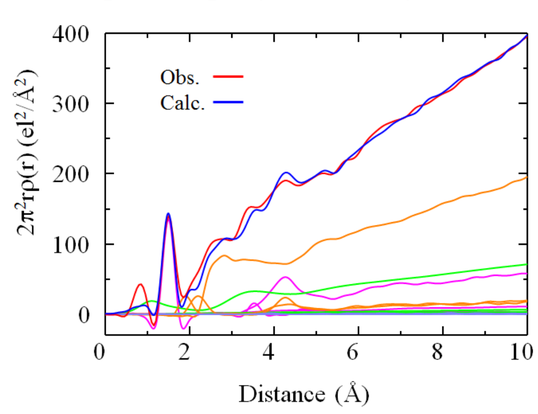
Unstable Mn^{3+}

$2Mn^{3+} + 2H_2O \rightleftharpoons Mn^{2+} + MnO_2\downarrow + 4H^+$



A schematic diagram of a redox flow battery

$89\ H_2O \cdot 3\ H_2SO_4 \cdot 1\ TiOSO_4 \cdot 1\ MnSO_4$



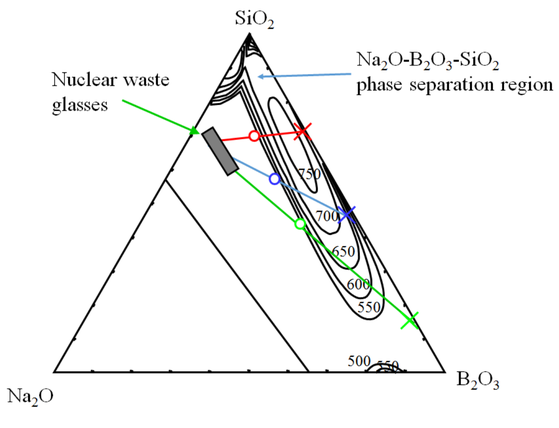
The experimental and calculated total correlation functions

♦ Chemical Durability and Phase Separation of Nuclear Waste Glasses

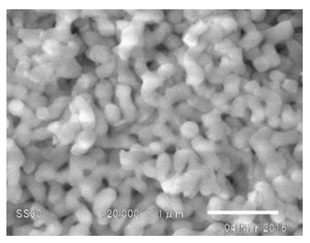
Control of the chemical durability of nuclear waste glasses

Nuclear waste glass

Composition	wt (%)	mol (%)
SiO_2	49	54
B_2O_3	15	14
Na_2O	10	11
Li_2O	3	7
CaO	3	4
Al_2O_3	5	3
ZnO	3	3
FP	12	4

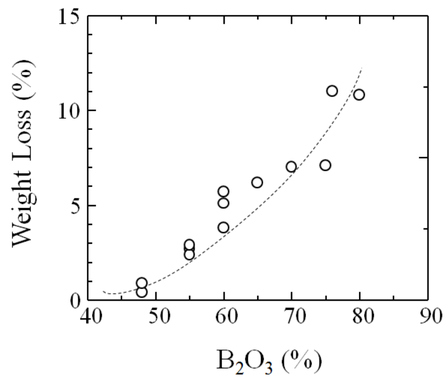


$10Na_2O \cdot 50B_2O_3 \cdot 40SiO_2$



SEM photograph after phase separation and elution

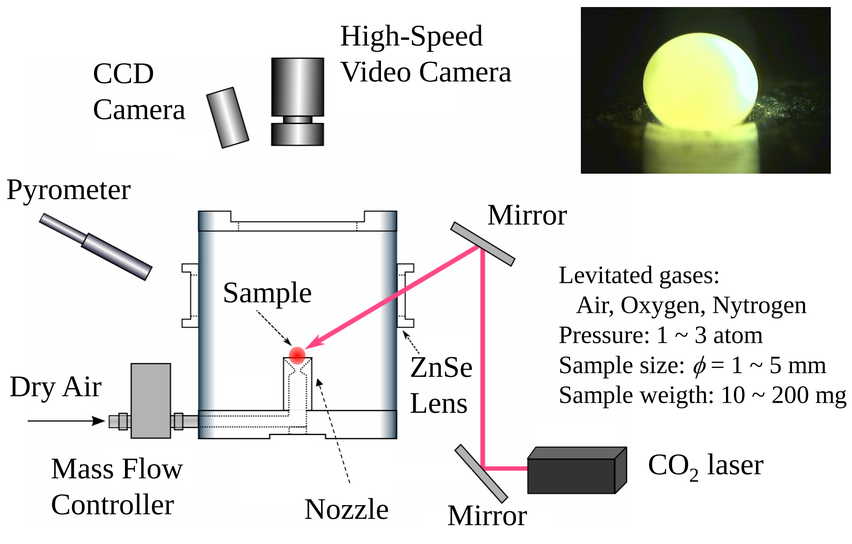
Na_2O-B_2O_3-SiO_2-Li_2O-Al_2O_3-CaO-ZnO-ZrO_2

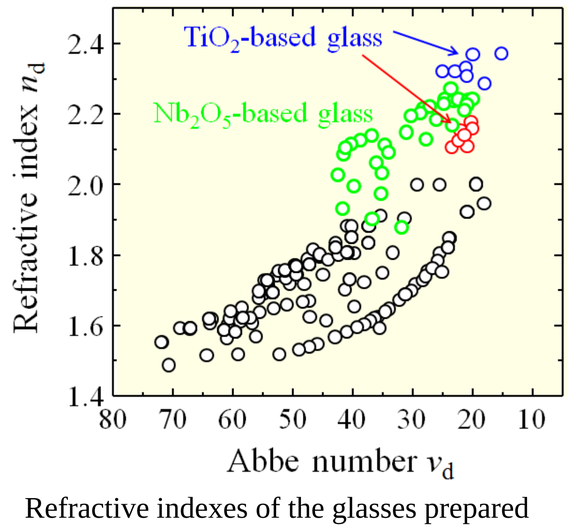


Weight loss after phase separation and elution

♦ Glasses prepared by using gas levitation furnace and their physical properties

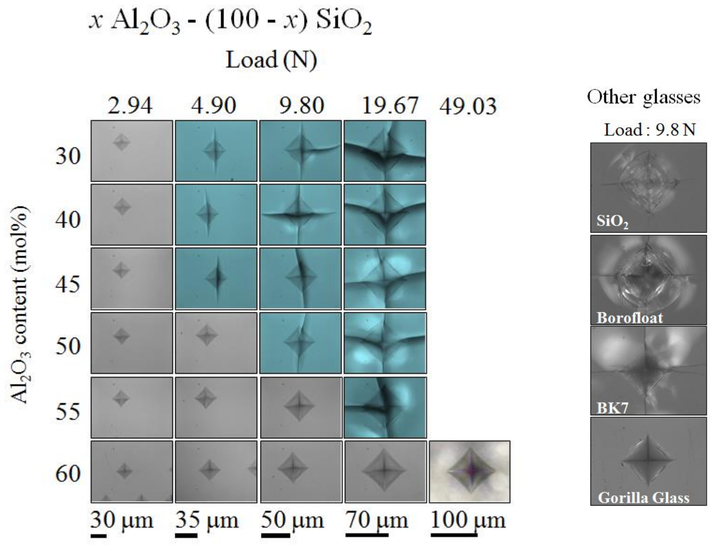
Gas levitation furnace





Refractive indexes of the glasses prepared

$x\ Al_2O_3$ - $(100 - x)\ SiO_2$



Mechanical properties of the glass prepared