Usage Report for Fiscal Year 2020

Project Title:

Structure and properties of multi-component oxides

Name:
○**Nguyen Van Hong(1), Toshiaki Iitaka(2)**

Laboratory at RIKEN:
(1) RIKEN Cluster for Pioneering Research, Theoretical Quantum Physics Laboratory
(2) RIKEN Center for Computational Science, Discrete Event Simulation Research Team

1. Background and purpose of the project, relationship of the project with other projects

Disordered networks with flexible structure are at the heart of a multitude of materials with functional properties. For example: The network structure of the SiO_2-Al_2O_3-ZrO_2-CaO based glass system is used in the hazardous waste treatment technology; The network structure of the SiO_2-P_2O_5 based glass system is the decisive factor to make bioactive materials ; The glassy network structure based on SiO_2-P_2O_5-V_2O_5-B_2O_3-SeO_2-TeO_2 containing Li is applied to create ionic conductive materials. Glass systems based on silicate and boro-silicate networks (Na_2O-B_2O_3-SiO_2 and K_2O-MgO-SiO_2) are used in fiber optic fabrication. Establishing the glassy network structure, and its relation to the physical-chemical and photo-electronic properties through the principle of rational design is a prerequisite for making new functional materials. We apply molecular dynamism and monte-carlo simulation method (atomic level simulation to investigate the fundamentals of basic networks; the influence of material composition on the basic network structure; influence of technological conditions (temperature, pressure, cooling rate, annealing time) on the network structure. Network-forming materials with different bonding mechanisms (SiO_2; GeO_2; SiO_2-Na_2O_3; SiO_2-CaO; SiO_2-MgO; SiO_2-P_2O_5-CaO; SiO_2-Al_2O_3-CaO; B_2O_3-Al_2O_3-SiO_2 ; SiO_2-P_2O_5-Al_2O_3…) will be investigated in this project. The above-mentioned oxide glass systems are materials containing typical network-forming oxides (SiO_2, GeO_2, P_2O_5, B_2O_3) with different bonding mechanisms which will create different network structure with different characteristics. This is the basis for making functional materials with desired properties. Structural information and the relationships between network structures and corresponding properties of glass oxide systems is the key data for designing new materials. Properties will be controlled through structure. Controlling the topology of network structure by changing the fabrication technology conditions or changing the composition ratio of functional oxides (network oxide, network structure oxide, intermediate oxide) will help to create materials with the desired structure and functional properties. This is also the purpose of this research.

2. Specific usage status of the system and calculation method

Molecular dynamics simulation, data mining, and visualization method are applied to clarify the structure and properties of multicomponent-oxide systems:

3. Result

Topology of SiO_x units and glassy network of magnesium silicate glass at different pressures are investigated by molecular dynamics simulation to clarify its microstructure under compression. The investigation results have been published on 01 papers

4. Conclusion

The form of SiO_5 and SiO_6 polyhedra is almost not changed under compression. However, the SiO_4 tetrahedra is distorted as pressure increases. At ambient pressure, the –Si–O– glassy network in Mg_2SiO_4 glass is split into subnets/clusters. Under compression, the subnets/clusters tend to merge each other forming larger subnets/clusters. The degree of polymerization of –Si–O– network increases with pressure. There is a tight correlation between the PRDFs and corresponding BADs, BLDs. The Si–Si, Mg–Mg, Si–Mg and O–O distances can be determined via

corresponding BADs and T–O BLDs. The formation of edge- and face sharing bonds between SiO_x units at high pressure is the cause of the frst peak splitting of Si–Si PRDF. The correlation between the microstructural characteristics (BAD, BLD) and the peaks of PRDFs support us a method to determine the microstructural change of Mg_2SiO_4 glass under compression. The number of corner-, edge- and face sharing Si–Si bonds increases as pressure increases. They are not uniformly distributed in model but forming clusters. The clusters of face-sharing Si–Si bond clusters are small and very stable. These face-sharing Si–Si bond clusters are considered as rigid-particles (or hard particle). The –Si–O– glassy network comprises the rigid-particles of face-sharing Si–Si bonds embedding in mixture network of corner- and edge-sharing Si–Si bonds. The Mg^{2+} ions tend to link to –Si–O– glassy network via NBOs (at low pressure) and via both NBOs and BOs (at high pressure). Mg^{2+} ions can incorporate in –Si–O– glassy network via corner-, edge- and face sharing Mg–Si bonds. These bond types are not uniformly distributed but forming clusters. It also exists the Mg-rich regions in model of Mg_2SiO_4 glass. This demonstrates the structural and compositional heterogeneities in magnesium silicate glass.

5. Schedule and prospect for the future

In next time, we will focus on the structural investigation of waste storage materials and bioactive materials based on network-forming oxides: B_2O_3, Al_2O_3, SiO_2, P_2O_5... These are typical groups of nuclear waste storage materials and bioative-materials with many good properties.

6. If no job was executed, specify the reason.

Usage Report for Fiscal Year 2019

Fiscal Year 2020 List of Publications Resulting from the Use of the supercomputer

[1] N. H. Son, N. H. Anh, P. H. Kien, Toshiaki Iitaka and N V Hong, *Topology of SiOx-units and glassy network of magnesium silicate glass under densification: correlation between radial distribution function and bond angle distribution*, Modelling Simul. Mater. Sci. Eng. (2020) 28 065007, doi: https://doi.org/10.1088/1361-651X/ab9bb4.