JASMAC Conference of the Japan Society of Microgravity Appllication

P20

溶融塩中における酸化シリコンの融体構造

Melting Structure of Silicon Dioxide in Molten Salts

鈴木祐太 [1]，福中康博 [1]，後藤琢也 [1]，
Yuta SUZUKI[1], Yasuhiro FUKUNAKA[1], Takuya GOTO[1]
1　同志社大，Doshisha Univ.

Many studies[1-3] related to in-situ resource utilization (ISRU) have been conducted to separate and recover useful elements such as silicon from lunar regolith by molten salt electrolysis. Since SiO_2 is the main component of lunar regolith, it is beneficial to fabricate polycrystalline silicon films from SiO_2 on the moon as a material for solar cells. In the molten salt electrolysis, the solubility behavior of SiO_2 and electrochemical behavior of silicon ion is dependent on the composition of molten salt. Hence the understanding of the interactions between silicon ion formed by dissolving SiO_2 and constituent ions of the melt is important to control the solubility process of SiO_2 and the silicon electrodeposition process. Therefore, in this study[4-5], we report the melting structure of SiO_2 in fluoride melts, whose bath have several advantages, especially the ability to obtain crystalline silicon directly from SiO_2 at lower temperatures because of high solubility of oxides, by combining Raman spectroscopy and DFT calculation.

We investigated melt structures of eutectic LiF-KF, LiF-NaF and NaF-KF adding SiO_2 through Raman spectroscopy and density functional theory calculations. The interactions between silicon ion and constituent ions of the fluoride melts have been identified. A good agreement was observed between the calculated and experimental Raman spectra for the melts. The spectra were characterized by two kinds of coordination structures: ion-like structure such as $SiF_2O_2^{2-}$ and $Si_2O_5^{2-}$; and molecule-like structure such as SiF_3O-Li and SiF_2O_2-2Li (**Fig.1**). Moreover, when Li_2O as a source of O^{2-} was added, remarkable bands appeared which were attributed to ion-like structure of $SiFO_3^{3-}$ and SiF_3O^-, indicating that O^{2-} ions have potential to promote the formation of oxyfluoride monomers by cleaving the Si-O-Si bands of $Si_2O_5^{2-}$ ions or SiO_2. The information for the coordination structure around silicon ion in the fluoride melts are important towards electrodeposition process of silicon films from lunar regolith in terms of designing the electrolyte.

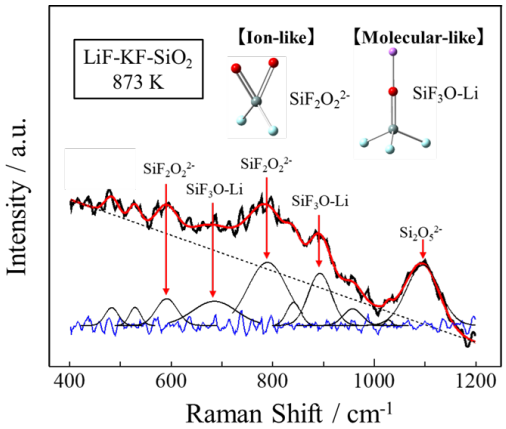

Fig. 1　Raman spectra of LiF-KF melt adding 5.0 mol% SiO_2. Raw data (black bold line), fitting curve (red line), base line (dotted line), residual curve (blue line) and separated bands (black lines). The inserted molecular models are optimized structures of silicon oxyfluoride monomers by DFT calculations.

References

1) G. S. Jackson, S. Elangovan, and P. E. Hintze: Electrochem. Soc. Interface **29** (2020) 65.
2) D. Kornuta, A. Abbud-Madrid, J. Atkinson, J. Barra, G. Barnhard, D. Bienhoff, B. Blair, V. Clarkg, J. Cyrus, B. DeWitt, C. Dreyer, B. Finger, J. Goff, K. Ho, L. Kelsey, J. Keravala, B. Kutter, P. Metzger, L. Montgomery, P. Morrison, C. Neal, E. Otto, G. Roesler, J. Schier, B. Seifert, G. Sowers, P. Spudis, M. Sundahl, K. Zacny and G. Zhu: REACH-Rev. Human Space Expl., **13** (2019) 100026.
3) T. Goto, Y. Sakanaka, A. Mutrata, K. Iwami, and T. Ishikawa: Space Utiliz. Res., **30** (2016) 1.
4) Y. Suzuki, T. Park, K. Hachiya, T. Goto: J. Fluorine. Chem., **238** (2020) 109616.
5) Y. Suzuki, Y. Inoue, M. Yokota, T. Goto: J. Electrochem. Soc., **166** (2019) D564.