

京都大学若手人材海外派遣事業 スーパージョン万プログラム
研究者派遣プログラム

英文報告書

提出日：平成 27 年 4 月 20 日

1. 渡航者 (日本語)			
氏名	北田 敦	採択年度	H26
部局	工学研究科	電話	-----
職名	助教	メール	
研究課題名	シェブレル高圧相の電池正極材料への応用		
海外渡航期間	平成 26 年 4 月 28 日～ 平成 27 年 3 月 27 日		
渡航先 (英語表記)	国名：United Kingdom 大学等研究機関名：University of Edinburgh 研究室名等：J. Paul Attfield Lab. 受入研究者名：Prof. J. Paul Attfield		
2. 渡航の報告 (英文)			
渡航先の研究環境、研究者との交流、研究発表の状況等、渡航中の滞在経験について英語 (500～1000 語) で記述して下さい。受入研究者と撮影した写真や研究発表で用いた図等について、可能な範囲で別添として提出して下さい。ページ数については増加してもかまいません。			
<p>Prof. J. Paul Attfield Lab, where I stayed in University of Edinburgh, has a high-pressure apparatus with multi-anvil type, which realizes an extreme reaction condition, i.e. high pressure (~20 GPa) and high temperature (~1400 °C). 20GPa corresponds to the pressure at ~600 km deep from the Earth's surface. The advantage of the high-pressure machine is its ability to quench sample to ambient pressure. Such sample with high-pressure phase has larger density than that with ambient-pressure phase. This means that smaller space for ion-conduction, but it in turn gives higher electrode potential. This is why I chose Edinburgh, which is the best place to try synthesis and characterization of high-potential positive electrode materials.</p> <p>Using the high-pressure machine I tried two kinds of research themes. What I have chosen for seeking high-pressure structural transitions are trimolybdenum tetrasulphide (Chevrel phase, Mo₃S₄) and lithium manganese oxide (LiMn₂O₄). Both compounds are famous as positive electrode materials for lithium and/or magnesium ion secondary batteries. I found high-pressure phase of Mo₃S₄ exists and can only be obtained only at 11GPa, 1200 °C, although I could not obtain it as major phase. By contrast, high-pressure phase of LiMn₂O₄ was successfully obtained as major phase at 6 GPa, 900 °C. I studied on room temperature lithium extraction from high-pressure phase of LiMn₂O₄. As a result, via oxidation the original Mn-O framework transformed into spinel-type framework. It is surprising from the fundamental viewpoint that such inorganic system transforms at room temperature. These high-pressure works need further</p>			

investigation, and Prof. Attfield is willing to collaborate with me.

Apart from high-pressure synthesis, I also investigated lithium extraction from a lithium titanium oxide (LiTi_2O_4). Different from common oxidant such as bromine and iodine, I found that water can be used as a gentle oxidant. The obtained $\text{Li}_{0.33}\text{Ti}_2\text{O}_4$ has no impurity, which enable us to determine its crystal structure for the first time. By analyzing the powder X-ray diffraction and neutron diffraction profiles I found that even at room temperature migration of Ti atoms occurred in accordance with the lithium extraction, the degree of which has quantitative relationship with the amount of the lithium deficiency. Prof. Attfield and I made fruitful discussion about crystal structure and migration mechanism of $\text{Li}_{0.33}\text{Ti}_2\text{O}_4$, and the results are now submitted to high-profile RSC journal Chemical Communications. LiTi_2O_4 is known as a negative electrode material, when lithium is intercalated into LiTi_2O_4 . In the case of lithium extraction, however, the electrode potential of $\text{Li}_{0.33}\text{Ti}_2\text{O}_4$ was found to be $\sim +3$ V vs. Li, suggesting potential use as a positive electrode material.

I had an opportunity to have a seminar for School of Chemistry in Edinburgh (Thu 27 Nov 2014, 1 hour; <https://www.csec.ed.ac.uk/seminars>.) In my talk I focused on chemical modification of layered compounds including my own works. After seminar Dr. Mark de Vries, a lecturer in School of Chemistry showed much interest in magnetic properties of my compounds, since he majors in quantum magnetism of two-dimensional compounds (e.g. *Nature* 468, (2010) 908). We enjoyed our deeper discussion and we decided starting-up collaboration.

Consequently, I developed close and amicable relations with high-profile researchers in Edinburgh during my stay. I am really grateful to Edinburgh and I believe that I carried out my research mission successfully.