

# High-throughput cathode materials exploration by combinatorial technology

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Concept of combinatorial chemistry was proposed by Prof. Robert B. Merrifield who designed efficient solid phase peptide synthesis using polymer beads in 1960s. On the other hand, around the same time, J.J. Hanak, K. Kennedy et al. also reported the other concept of combinatorial metal and inorganic materials exploration using sputtering technique and so on. One of reasons why combinatorial metal and inorganic materials exploration didn't developed in 1960s was due to difficult to establish computer automation. From 1990s, however, many researcher tried to establish high-throughput materials exploration system since we could easily use personal computer.

Our research group (NIMS: 1999-2006, TUS: 2003-present) have hitherto developed combinatorial high-throughput preparation system based on solution processing. From the beginning, we are exploring various kinds of cathode materials for lithium ion secondary battery using our robot system. And, in order to accelerate materials exploration, we made not only the preparation system but also high-throughput powder X-ray diffractometer for phase identification and the combinatorial electrode array for obtaining 1<sup>st</sup> charge-discharge capacity.

As one example, multi-elements substituted layered-type  $\text{Li}(\text{Ni},\text{Co},\text{Ti})\text{O}_2$  were prepared using our exploration system. The following figure shows pseudo-ternary  $\text{Li}_2\text{O}-\text{NiO}-\text{CoO}_{1.33}-\text{TiO}_2$  reaction phase diagram at  $700^\circ\text{C}$  under air atmospheric condition. From this diagram, it was found that the composition ratio of layered-type structure was  $\text{Li} : (\text{Ni},\text{Co},\text{Ti}) = 1:1$ . And,  $\text{Li}(\text{Ni},\text{Co})_{0.9}\text{Ti}_{0.1}\text{O}_2$  compounds were better cycle performance than the other  $\text{Li}(\text{Ni},\text{Co},\text{Ti})\text{O}_2$ . In this joint seminar, I will also show the other results of cathode materials exploration.

