8 Element Strategy Initiative to Form Core Research Center for Electron Materials

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8-1 Introduction

Japan is reliant on imported supplies of actinide and rare-earth elements from other countries. Thus, there is a risk of a supply shortage of rare elements induced by the export control policy of resource-rich countries and the rapid increase in global demand for these elements. It is therefore necessary to develop functional substances using common elements rather than rare elements. To create a strong position in materials science amid fierce competition, the national "Element Strategy Project" was started in 2012. This project designates four areas of direct competition for Japanese industry: electronic, magnetic, battery, and structural materials. We are aiming to develop entirely new materials that do not use rare elements, which requires collaborative research in each area on the following: (1) material creation, (2) theory of electronic state, and (3) analysis and evaluation.

For electronic materials, the Tokyo Institute of Technology (representative supervisor: Prof. Hideo Hosono) was chosen, deputy base of the material evaluation and analysis the KEK (agency supervisor: Prof. Yoichi Murakami). In the Tokyo Institute of Technology for element strategy "TIES", we are developing a material open based on successful experience far away from development policy, and are pioneering electronic materials to create new guidelines for material design, and then by making a material for practical use in the harm less elements it is intended to open up new material science. To achieve this goal, with the support of theoretical calculations advanced evaluation technology, we and are developing an effective system for creating new high-performance electronic materials containing no toxic substances. In the KEK deputy base, we are researching the electronic and magnetic structures of the system, and precisely determining the local structure of light elements such as hydrogen and oxygen in materials synthesized by the Material Creation Group by using synchrotron radiation and neutron scattering. The precise electronic structure of the interface and ultra-thin film also can be observed and evaluated by visualizing the depth distribution of electronic and chemical states. We will establish new techniques to determine the magnetic phase diagram, the degree of spin freedom, and the charge state, and measure the stable position of hydrogen by using muons.

8-2 Organization of the alliance

Figure 1 shows the organization chart of KEK / IMSS. IMSS is made up of three research systems: synchrotron radiation science, neutron science, and muon science. In each system, to develop the beam line and experimental equipment, we support research on quantum beam science by generating a radiation-neutron-muon. The IMSS Center consists of the Condensed Matter Research Center (CMRC) to promote advanced research by using complementary / concerted quantum beams. The CMRC plays a central role in the Elemental Strategy Project. Four researchers in the CMRC will conduct research as Principal Investigators (PI) of TIES. The researchers specialize in electronic state analysis using dynamic structural analysis and precision structural analysis by soft X-ray, VUV, X-ray, neutrons, and muons. The PIs are conducting research in cooperation with researchers in TIES and many others in KEK.



CMRC plays a central role in element strategy project

Fig. 1: Organization chart of the Institute of Materials Structure Science (IMSS) in the High Energy Accelerator Research Organization (KEK).

8-3 Features of the alliance

It is rare for a single institute to own multiple quantum beams of synchrotron radiation, neutrons, and muon-positrons. Synergies arising from the use of multiple probes will produce significant results in basic science. The Element Strategy Project will use quantum beams to develop new materials. In this project, quantum beam experts cooperate closely with theorists and materials creators to create a new paradigm of materials research and development.



Fig. 2: Research facilities of synchrotron radiation, neutrons, and muons in KEK / IMSS. These will be used in the Element Strategy Project.

8-4 Facilities of the alliance

Figure 2 shows the research facilities of synchrotron radiation, neutrons, and muons in KEK / IMSS. There are laboratory equipment and beamlines in many of these facilities, but the following beamlines have a strong track record in materials science research and so will be used in this Element Strategy Project.

In the PF and PF-AR, crystal structures can be measured precisely in BL-8A and -8B, reciprocal space can be investigated in BL-3A and -4C, and the structure analysis of thin-films can be performed in BL-2C and -16A. Furthermore, a structural analysis beamline is being prepared by using high-energy X-ray at PF-AR. In J-PARC KENS, we can measure high-resolution powder diffraction on SHRPD, high-intensity powder diffraction on NOVA for precise structural analyses, and inelastic scattering by HRC. In addition to the



general-purpose μ SR beamline, the J-PARC MUSE U-line will be available for ultra-slow muons in the near future.

8-5 Future of the alliance

Figure 3 shows the cycle of precise structure analysis of new materials made possible by effective use of the quantum beam devices in KEK for cooperation TIES. At the same time as the creation of new materials, fine structure analysis using synchrotron radiation X-ray, electronic structure analysis using VUV and soft X-ray, measurement and analysis of the dispersion relation of magnons and phonons and (magnetic) structure analysis using neutrons are conducted. In the future, we will build a system to rapidly analyze local electronic state using muons, thus contributing to the discovery of new electronic materials by high-speed measurement of the new materials created.



Fig. 3 Material, design, and characterization cycle in KEK.