

MATERIALS SCIENCE:



Ajisai"- *Hydrangea*

The argument that the nature of matter originates from the type and arrangement of atoms is widely accepted. Conventional structural analysis, however, has done little to connect structural information directly with macroscopic properties of materials. High brilliance, low emittance and highly polarized synchrotron radiation (SR) provided by SPring-8 is now being applied to elucidate the direct relationship between them. Successful applications in this year are widely distributed among research fields on superconducting, structural, hydrogen-storage, strongly correlated, glass, and soft materials.

In the superconducting materials with the layered structure, it had been considered that the substitution of the primary element with other ones is baneful to superconductivity. Nohara *et al.* overturned this common sense: they discovered a high- T_c iron-based superconductor by substituting Pt for a large portion of the primary element of Fe. They also observed two types of superconducting phase due to the bistable valence states of As ions, As^{3+} and $[As_2]^{4+}$, in the newly discovered $Ca_{10}(Pt_nAs_8)(Fe_{2-x}Pt_xAs_2)_5$ ($n = 3,4$) system.

The difference in valence is directly related to the ionic size. Azuma *et al.* exploited this feature of the macroscopic structural property. They found colossal negative thermal expansion (CNTE) in the perovskite $BiNiO_3$ compound at high pressure and/or high temperature, which originates from the valence change from Ni^{2+} to Ni^{3+} owing to charge transfer between Bi and Ni ions. By tuning the transition temperature and pressure through the substitution of Bi with La, they succeeded in realizing CNTE under ambient conditions.

STRUCTURE

The increase in the ionic size can also be used as evidence of hydrogen absorption. Matsuoka *et al.* have clarified that EuH_x , which was considered to be different from other rare-earth metal hydrides RH_x , is no longer an irregular member of the rare-earth metal hydrides. They conducted high-pressure diffraction and Mössbauer experiments in the EuH_x system, and found that the phase-transition sequence in EuH_x is similar to those of other RH_x systems. In systematic analyses, a small but non-negligible increase in the lattice constant, indicating a valence change in Eu through hydrogen absorption, was one of the key pieces of evidence supporting their conclusion.

Not only the number of electrons (valence) but also the orbital degree of freedom can now be examined by a sophisticated SR measurement technique. Ishii *et al.* developed polarization-analyzed resonant inelastic X-ray scattering (RIXS) for the first time, and succeeded in observing selectively the excitation between the e_g orbitals, corresponding to the orbital degree of freedom, from two types of excitations in a typical orbital order material, KCuF_3 . The nature of orbital ordering will be unveiled by this new approach.

Reverse Monte Carlo analysis combined with density functional theory has become one of the most powerful tools for discussing the unique local and intermediate-range structures that govern the physical properties of non-periodic systems. Kohara *et al.* interpreted the glass forming ability from the viewpoint of cavity and ring distribution in glasses. Furthermore, they found that the local environment around the atoms in MgO-SiO_2 glass shows wide variation, depending on both the coordination number and bond strength, which is the origin of the discrepancy between the interpretations based on X-ray diffraction and NMR.

The small-angle X-ray scattering (SAXS) measurements shed light on the development of functional polymers and soft materials on the basis of their chemical properties and hierarchical structures. Takahara *et al.* found that electrostatic interaction of one of polyelectrolytes, so-called PMTAC, strongly depends on the concentration of hydrated ions without significant change in the conformation, as revealed by SAXS analysis, and succeeded in fabricating a reversible and solvent-free adhesion system using its novel characteristics.

Structural analysis is a basic method for the characterization of materials, and is still being developed by cutting-edge SR technologies and many analytical approaches in order to gain deeper insight into materials science.

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