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Structural response to pressure in 1111-type iron-based superconductor $LaFeAsO_{1-x}H_x$

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Iron-based superconductor (iron pnictides) and cuprates are most well-known types of superconductor with critical temperature (T_c) higher than 50 K. In iron-based superconductors, the relation between the maximum Tc and structural parameters of FePn4 (Pn = pnictide) has been proposed as follows: the highest Tc is achieved when the Pn-Fe-Pn bond angle (αPn-Fe-Pn) approaches 109.5° as in a regular tetrahedron of FePn4 or when the Pn height from Fe plane (h_{Pn}) ~ 1.38 Å. The application of pressure is a direct and clean way to modify the local geometry of $FePn_4$ without the degradation of the crystal in comparison to the chemical substitution; hence, the detailed crystal structure under pressure warrants further investigation. A systematic study of the crystal structure of a layered iron oxypnictide $LaFeAsO_{1-x}H_x$, with a unique phase diagram of two superconducting phases and two parent phases, as a function of pressure was performed using synchrotron X-ray diffraction. We established that the $\alpha_{As\text{-}Fe\text{-}As}$ widens on application of pressure due to the interspace between the layers being nearly infilled by the large La and As atoms. This behavior implies that the $FeAs_4$ coordination deviates from the regular tetrahedron in our systems, which breaks a widely accepted structural guide albeit the increase of Tc from 18 K at ambient pressure to 52 K at 6 GPa for x = 0.2. In the phase diagram, the second parent phase at x ~ 0.5 is suppressed by low-pressure at ~1.5 GPa in contrast to the first parent phase at x ~ 0, which remains robust to pressure. We suggest that the spin/orbital fluctuation from the second parent phase gives rise to the high-T_c under pressure. The pressure responses of the FeAs4 modification, the parent phases, and their correlation are previously unexplained peculiarities in 1111-type iron-based superconductors.

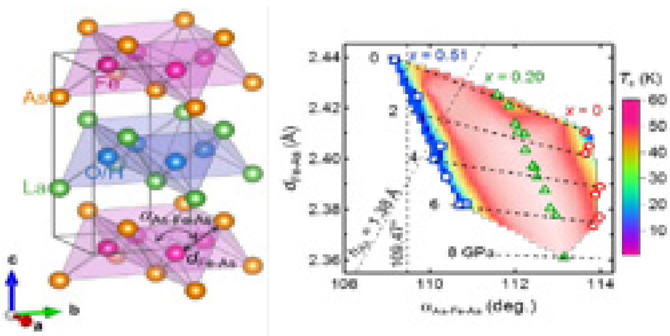

Figure1: Crystal structure of $LaFeAsO_{1-x}H_x$ and the contour plots of T_c as a function of As-Fe-As bond angle (αAs-Fe-As) and the Fe-As bond length (dFe-As).

Biography

Kensuke Kobayashi has received his doctor's degree in science from Osaka City University in 2009. Since April 2010, he has been a researcher at Condensed Matter Research Center (CMRC), Institute of Material Structure Science, KEK. At present, he is a Project Assistant Professor (MEXT Element Strategy Initiative) and worked on experimental studies of the structural and electrical properties of materials by means of synchrotron X-ray diffraction under external fields, such as pressure, electric field and low temperature

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