【Grant-in-Aid for Scientific Research(S)】

Integrated Science and Innovative Science (New multidisciplinary fields)

Title of Project : Development of High-brightness and High-intensity Positron Diffraction and its Application to Surface Studies

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Research Area : New multidisciplinary fields
Keyword : Electron・positron, Methodology

【Purpose and Background of the Research】

Low-energy electron diffraction (LEED) and reflection high-energy electron diffraction (RHEED) are important methods for determining the atomic geometry of material surfaces. We develop their positron (antiparticle of the electron) counterparts - low-energy positron diffraction (LEPD) and reflection high-energy positron diffraction (RHEPD) - to be used for surface structure analysis. Positron diffraction is easier to interpret as: (1) the exchange interaction with electrons is absent; (2) the surface sensitivity is high because the inelastic scattering cross section for the positron is high and the crystal potential for the positron is positive; and (3) the scattering factor for the positron falls off smoothly as that of X rays because it is repelled by the nuclei. Thus, positron diffraction can be used to analyzes surface atomic geometry with a high reliability. We also develop methods to determine the position of the atoms on the surfaces directly.

【Research Methods】

Since the positron is an antiparticle and so not found in everyday life, it is difficult to make a high-brightness and high-intensity beam. We make use of a high-intensity slow-positron beam at the Institute of Materials Structure Science, KEK, and enhance its brightness. The issues to be solved with the apparatus include: (1) the determination of the atomic geometry of the surfaces of topological insulators, which are known to be difficult to analyze with electron diffraction; (2) the determination of the positions of the atoms of heavy elements on the surfaces showing giant Rashba effect, paying attention to the height of the heavy atoms relative to the substrate surface; and (3) the analysis of the formation of the charge density wave and the metal-insulator transition accompanied by the Peierls transition, in which heavy elements also play significant roles. The direct determination of the atomic geometry is attempted in two ways: by analyzing the RHEPD patterns taken under various conditions with the Patterson function, and by using the holographic reconstruction of the atomic arrangement using the LEPD spectra taken at various energies.

【Expected Research Achievements and Scientific Significance】

The features of the surfaces of topological insulations and giant Rashba sufaces are expected to have significant consequences in the development of next-age electronic applications such as spintronics, energy-saving elements, and quantum computers. Investigations of the electronic structures of these surfaces have been widely performed with angle resolved photoelectron spectroscopy, etc. However, only a few studies of the atomic geometry of the relevant surfaces have been reported. We will correlate the surface electronic structures to the atomic geometries, making it possible to explain the spin splitting of the energy bands and the appearance of new functions by the atomic arrangements. Patterson analysis and positron holography will make it possible to conveniently and reliably determine the structure of unknown surfaces directly from the diffraction data.

【Publications Relevant to the Project】

[1] I. Mochizuki, et al., Atomic configuration and phase transition of Pt-induced nanowires on a Ge(001) surface studied using scanning tunneling microscopy, reflection high-energy positron diffraction, and angle-resolved photoemission spectroscopy, Phys. Rev. B 85, 245438-1-6 (2012).
[2] Y. Fukaya, et al., Atomic structure of two-dimensional binary surface alloy: Si(111)-√21×√21 superstructure" Surf. Sci. 606, 919-923 (2012).

【Term of Project】 FY2012-2016

【Budget Allocation】 165,700 Thousand Yen

【Homepage Address and Other Contact Information】

http://pfwww.kek.jp/slowpos/