

Poster Presentation

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TRHEPD rocking curve analyses of Pt/Ge(001) and TiO₂(110) surfaces

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Recently, we developed new total reflection high-energy positron diffraction (TRHEPD) apparatus [1] on a beam line of the linac-based intense positron beam of the Slow Positron Facility at KEK, Japan. The high intensity allows us to install a brightness-enhancement section, which to observation of clear positron diffraction patterns for crystal surfaces under total reflection condition. In this work, we investigated the atomic configuration of Pt-induced nanowires formed on a Ge(001) surface [2] using the apparatus. By means of the diffraction intensity analysis based on the dynamical diffraction theory, or TRHEPD rocking curve analysis, a previously proposed theoretical model [D. E. P. Vanpoucke et al., Phys. Rev. B 77, 241308(R) (2008)], composed of Ge dimers on the top layer and buried Pt arrays in the second and fourth layers, was confirmed to be the fundamental structure of the nanowire. We also investigated the atomic configuration of a rutile-TiO₂ (110) surface. It is well known that the structure of this surface transforms its periodicity from (1×1) to (1×2) by elevating the sample temperature above ~1100 K, whereas the detailed structure is yet to be revealed. There is a longstanding controversy between the structure models proposed by scanning tunneling microscopy, low energy electron diffraction, surface X-ray diffraction, first-principles calculation with density functional theory results, etc. To solve the problem, we have measured TRHEPD rocking curves and determined the atomic arrangements of the topmost crystal surface [3].

[1] K. Wada, et al., *Eur. Phys. J. D*, 2012, 66, 37; *J. Phys.: Conf. Ser.*, 2013, 443, 012082, [2] I. Mochizuki, et al., *Phys. Rev. B*, 2012, 85, 245438, [3] I. Mochizuki, et al., in preparation

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