Electronic structure of Pt-induced nanowire on Pt/Ge(001) surface
studied by angle-resolved photoemission spectroscopy

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Self-assembled nanowires have attracted a great deal of interests as not only potential applications in nano-devices, but also fundamental understandings of one-dimensional properties. Defect-free nanowires with single-atom width are fabricated on a Ge(001) surface by an adsorption of Pt atoms [1]. Recently, van Houselt et al. [2] reported that the Pt-induced nanowires undergo a Peierls-type structural phase transition (SPT) around 80 K with scanning tunneling microscopy/spectroscopy (STM/S). We experimentally found out, by using reflection high-energy positron diffraction [3], that the atomic configuration is explained by the nanowire (NW) model [4] (Fig. 1), and that the SPT is derived from the height difference between the topmost Ge dimer atoms. However, the electronic band dispersions in the SPT are still unrevealed. In this study, we investigated the electronic structure of the Pt/Ge(001) surface by using angle-resolved photoemission spectroscopy (ARPES).

Well-defined Ge(001)-(4×2)-Pt surfaces with single-domain were prepared on vicinal Ge(001) substrates (2° OFF, n type, R < 0.3 Ωcm) tilted in [110] direction. Pt atoms were deposited on the clean Ge(001) surface for 0.9 monolayer (ML) at 720 K and following the Pt deposition for 0.3 ML at 620 K, where 1 ML corresponds to 6.3×10^{14} atoms/cm^2. The ARPES measurements were performed with a polarized radiation of hν = 25 eV at BL-18A and 19A beamlines of the KEK Photon Factory (Institute for Solid State Physics, University of Tokyo).

Figure 2 shows a typical STM image of the vicinal Pt/Ge(001) surface [5]. The Pt-induced nanowires, covering a large area, are aligned in the [110] direction parallel to the step edges. The inset shows a low-energy electron diffraction (LEED) pattern from the vicinal surface. A long range order of the uniformly oriented p(4×2) structure is also confirmed by the LEED pattern.

Figures 3(a) and 3(b) show the ARPES images taken along the [110] direction at 65 K and room temperature, respectively [3]. In both images, the Ge bulk band appears at the center of the first surface Brillouin zone (SBZ) near the Fermi level.

The dispersions around the Ζ point within the bulk band gap are attributed to the surface state bands. The theoretical band dispersion for the NW model [4] indeed explains the observed dispersion at room temperature. According to the theory behind that
model, the band dispersion can be attributed to the bonding state between the topmost Ge dimers and the Pt atoms in the fourth layer as shown by the bottom Pt atoms in Fig. 1. At 65 K, this dispersion shifts to a deeper region that is about 0.2 eV below the Fermi level. The change in the band dispersion from 65 K to room temperature seems to be explained by the displacement of the topmost Ge dimer atoms [3].

However, if the SPT is derived from a Peierls transition, the width of a nesting vector at the Fermi level should appear to be 0.4 Å⁻¹ and not to be 0.8 Å⁻¹ as observed at the J point. Therefore, we consider, the shift of the band dispersion is due to the displacement of the topmost Ge dimers, but is not directly related to the Peierls instability.

To confirm the origin of the structural phase transition, more precise ARPES-based experiments are under progress [5].

![Fig. 3 Second derivatives of ARPES spectra obtained at (a) 65 K and (b) room temperature, respectively. The photoemission intensity is greater in the brighter areas in gray scale. The white vertical lines denote the Γ and J points.](image)

**References**

[5] K. Yaji et al., to be submitted.