Dispersive Resonance Bands within the Space Charge Layer of Metal-semiconductor Junction

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Based on measurements of angle resolved photoemission, we report that in the Pb/Ge(111)-$\sqrt{3}\times\sqrt{3}$ R30° structure, in addition to three bands resembling Ge bulk band edges, a fourth dispersive band resembling the non split off (NSO) band is found near the surface zone center. While three Ge bulk-like bands get distorted due to strong coupling between Pb and Ge, the NSO-like band gets weaker and disappears for larger thickness of Pb, which, when combined with ab initio calculations, indicates its localized nature within space charge layer.

In Fig. 1, we show the gray-scale representations of the photoemission results for the clean Ge(111) -c(2x8) surface (top), and Pb/Ge(111)- $\sqrt{3}\times\sqrt{3}$ R30 surface (bottom), respectively in two symmetry directions. Note that symbols on the top of the Fig. 2 represent the symmetry points for (1x1) surface brillouin zone,

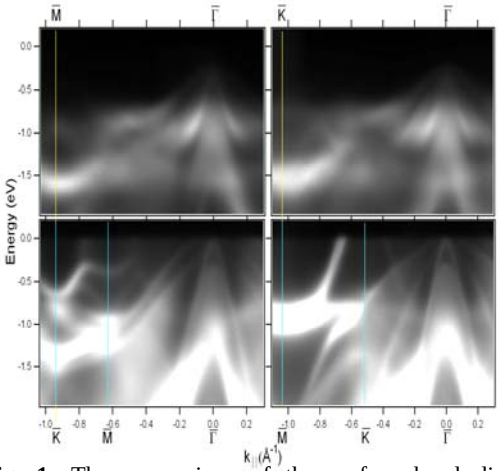

Fig. 1: The comparison of the surface band dispersions between Ge(111)-2x8 and Pb/Ge(111)$(\sqrt{3}\times\sqrt{3})R30^{\circ}$ surface.

while symbols at the bottom represent the symmetry points for $\sqrt{3}\times\sqrt{3}$ R30 surface brillouin zone. It is clear that in the photoemission results either for Ge(111)-c(2x8) or for Pb/Ge(111)- $\sqrt{3}\times\sqrt{3}$ R30, dispersive energy bands are observed about the symmetry points corresponding to the surface zone boundaries, as indicated by vertical bars. These bands are likely to originate from the surface structures.

Clearly, Fig. 2 shows a set of four new bands near the surface zone center in both symmetry directions in the Pb/Ge(111)-$\sqrt{3}\times\sqrt{3}$ R30° surface. These four new bands have neither correspondence to the energy bands in Ge(111) surface nor the energy bands in Pb/Ge(111)-$\sqrt{3}\times\sqrt{3}$ R30°, measured or calculated previously. However, at the first sight, those bands resemble the bulk hole band edges of Ge. Since the Ge(111) used in this experiment is highly doped n-type, the four new bands observed are possibly related to the doping effect from Ge(111). In Figs. 2(a) and (b), we superimposed the calculated Ge bulk band edges dispersing in the same symmetry direction (ΓK for bulk, $\bar{\Gamma}\bar{K}$ for 1x1, and $\bar{\Gamma}\bar{M}\bar{K}$ for $\sqrt{3}\times\sqrt{3}$ R30°) onto the 2D image data. As is evident, the calculated bulk band edges, HH, LH, SO (red dashed curves), and NSO (blue dot curves), match the measured four bands very well within the large energy range from Fermi level down to 1.0 eV. The photon energy dependent data, which is not presented in this paper, shows the energies of the four bands don't shift

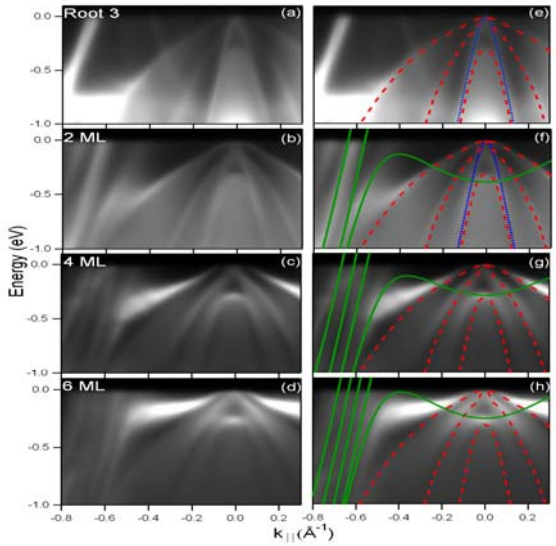

Fig. 2: Angle-resolved photoemission data presented as grey-scale images as a function of energy and $k_{||}$ for (a) Pb/Ge(111)-$\sqrt{3}\times\sqrt{3}$ R30°, and (b) 2 ML (c) 4 ML and (d) 6 ML of Pb on Ge(111)

with photon energies, indicating the surface related nature. Hence, it seems that the surface state becomes a surface resonance (SR), crossing the whole inversion layer and strongly mixing with bulk band edges. Similar results were observed by Tang *et. al.* [1] that the surface state of Ag thin film at the thickness smaller than its decay length presents the energy dispersions resembling HH, LH and SO band edges as a result of the strong interaction with Ge bulk edges.

[1] S.-J. Tang, T. Miller, and T.-C. Chiang, Phys. Rev. Lett. **96**, 036802 (2006).