Electronic versus Lattice Match for Metal-Semiconductor Epitaxial Growth: Pb on Ge(111)

It has been a long-standing puzzle for years that metal films can grow smoothly on semiconductor surfaces, retaining its own lattice constant, in spite of large lattice mismatch [1, 2, 3, 4]. In the past, scientists have either overlooked the reason or naively assumed that the large lattice mismatch caused the metal films to be free-standing-film-like. In a recent Phys. Rev. Lett. paper [5], Shu-Jung Tang of National Tsing Hua University, Hsinchu, Taiwan and co-workers reported the discovery of an important clue to this puzzle by investigating the system of Pb films on Ge(111). They showed that the growth of an incommensurate (1×1) parallel-epitaxy configuration is bound to another mysterious driving force for the epitaxial growth: electronic match. The perfect electronic match would cause the maximum hybridization between the quantum-well states (QWS) of the metal films and band edges of the semiconductor substrate so as to reduce the energy of the system.

The mismatch between the Pb and Ge lattice constants, 4.92 Å and 5.65 Å, is 13%. However, if the Pb film is rotated by 30º from the I(1×1) configuration, the Pb (2×2) unit cell and the substrate $\sqrt{3}\times\sqrt{3}$ unit cell become well matched (Fig. 1).

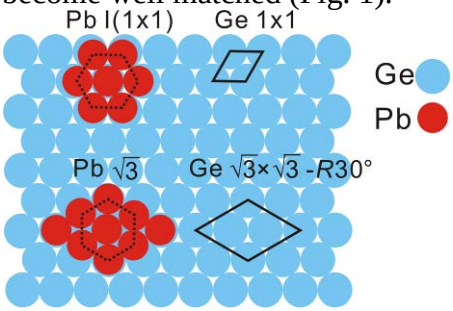

Fig. 1 Schematic diagrams for the Ge(111)-(1×1) substrate surface, a Ge(111)-(1×1) unit cell, a Ge(111)- $\sqrt{3}\times\sqrt{3}-R30°$ unit cell, a Pb I(1×1) domain, and a Pb $\sqrt{3}$ domain.

Low energy electron diffraction (LEED) measurements reveal the film growth orientation (Fig.2). Patterns from the bare Ge(111)-c(2×8) and the Pb/Ge(111) - $\sqrt{3}\times\sqrt{3}-R30°$ β phase establish the reference orientations and scale factors. Upon Pb coverage at 2 monolayers (ML), the $\sqrt{3}\times\sqrt{3}-R30°$ pattern is suppressed. An attenuated Ge(111)-(1×1) substrate pattern remains and is accompanied by six short arcs with the same orientation but farther out. The radius of the arcs indicates an I(1×1) Pb overlayer. Also evident in the data is the emergence of $\sqrt{3}$ domains at 3 ML which eventually dominates at higher Pb coverages.

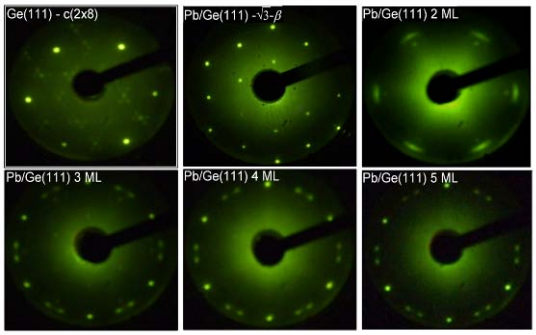

Fig. 2 LEED patterns, taken with the beam energy at 40 eV, from Ge(111)-c(2×8), Pb/Ge (111)- $\sqrt{3}\times\sqrt{3}-R30°$ β phase, and 2, 3, 4, and 5 ML of Pb overlayers.

Angle-resolved photoemission mapping of Pb overlayers of thicknesses 2, 4, 6, 8, and 15 ML along the $\bar{\Gamma}\bar{K}$ direction yield spectral functions shown in Fig. 3. At 2 ML, the results closely resemble the *k*-resolved one-dimensional density of states of the Ge bulk band structure because of a strong hybridization of the Pb and Ge states and the large contribution from the Ge states within the photoemission probing depth [6].

The data at higher coverages (4-15 ML) in Fig. 4 are quite different; an Anderson model involving a hybridization interaction of the discrete Pb QWS subbands and the Ge states [5 錯誤! 尚未定義書籤。] is used to construct a model spectral function. The solid purple curve shows $E_q(k_{\square})$, the dispersion of the "bare" QWS subband.

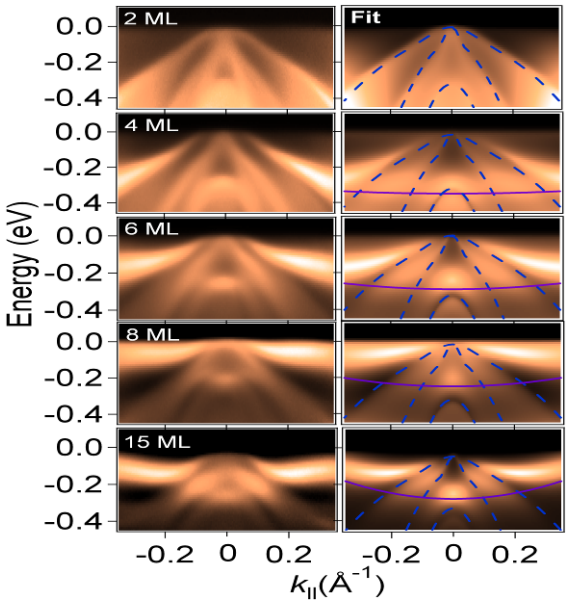

Fig. 3 Left panel: angle-resolved photoemission results along $\overline{\Gamma}\overline{K}$ for Pb film thicknesses of 2, 4, 6, 8, and 15 ML. Right panel: model fits to the data. The dashed curves indicate the Ge band edges. The solid curves indicate QWS subbands from the fits.

Two competing factors are at play: one is the interfacial energy, which is independent of the film thickness and favors the $\sqrt{3}$ lattice-matched configuration, and the other is the electronic energy associated with quantum confinement, which diminishes as $1/N$ and also depends on the degree of electronic hybridization across the Pb-Ge interface. A strong hybridization as a result of electronic match minimizes the effects of confinement, leading to a lower system energy. The authors convincingly argue that the I(1×1) configuration presents a much better electronic match than the $\sqrt{3}$ configuration based on general symmetry considerations. Thus, the I(1×1) configuration is preferred at small thicknesses for Pb/Ge(111).

The general understanding established in Tang, *et al.* [5], is important for devising strategies for smooth film growth with prescribed configurations – a key issue relevant to thin film electronics.

Reference:

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