Both for fundamental studies and for potential applications, it is oftentimes desirable to be able to grow uniform films in a layer-by-layer fashion on a substrate of different material. The interface with the substrate is an important factor controlling the nature of film growth. Generally, epitaxial growth of thin films is facilitated by a lattice-matched starting substrate, as there is a tendency for the substrate to serve as a template for further crystalline growth of the film. In typical cases there exists lattice mismatch which must be accommodated by strain or by the development of crystal imperfections in the substrate, film, or at the interface; consequently it may be more difficult to achieve layer-by-layer growth in these systems. Similar problems may be caused by reconstructions of the substrate surface, which may be quite complex. In these cases, it may happen that the presence of a third species at the interface can facilitate a desired growth pattern.

Ag films grown on the Si (111) surface provide examples of these issues. The equilibrium (111) Si surface has the well-known, but complicated, (7x7) reconstruction. Ag and Si both have fcc as their basic lattice but have large lattice mismatch with each other (Si: a= 5.43 Å, Ag: a= 4.09 Å). Depending on growth conditions, Ag on this surface can form flat or three-dimensional islands, or strained epitaxial layers. In the current work, we use Au to produce a commensurate Au/Si(111)-\(\sqrt{3} \times \sqrt{3}\) reconstructed surface as a seed layer before depositing Ag films. This has the effect of simplifying the surface reconstruction as well as modifying its chemical properties [1]. Subsequent growth of Ag films of various coverages was carried out at -165°C, and the films were annealed to RT. The electronic structure of the Ag thin film was probed by angle resolved photoemission using the high-resolution low energy synchrotron beam provided by U1-NIM beamline at SRC.

Figure 1 shows a series of energy distribution curves at normal emission from Ag films on Au/Si -\(\sqrt{3} \times \sqrt{3}\) at coverages ranging from 6 to 22 monolayers (ML). Each spectrum shows a series of discrete peaks representing the states of the quantum well formed by the thin metallic film. As is evident, the quantum well states peaks become narrower and shift to lower binding energies as the Ag film coverage increases. This coverage dependent behavior of the quantum well states can be simply explained through the phase accumulation model. The appearance of the intense and sharp Ag surface state near Fermi level is significant as it not only reflects good crystallinity of the film but also the important role of the intermediate \(\sqrt{3} \times \sqrt{3}\) seed layer in reducing the strain in the Ag film. This is because in films grown without the seed layer, the strain due to the Ag/Si lattice mismatch is known to significantly shift the initial state energy of
Ag surface state such that it moves above the Fermi level and becomes depopulated and significantly less intense [2].

Figure 2 shows the in-plane dispersion of the quantum well states and the surface state along the $\Gamma - K$ direction for a 22 ML thick Ag film. The bottom of the Ag surface state band is 26 meV above the Fermi level. A fit to the data (solid curve) reveals the effective mass $m^*/m$ of the surface state band to be 0.404 which is very close to the value 0.397 measured by F. Reinert et al [3] from the (111) surface of bulk Ag. The dispersions of the quantum well states (crosses) can be compared with those of Ag bulk bands calculated at constant $k_\perp$ (triangles) [4]. The match between the measurement and calculation is good for the quantum-well states with quantum numbers $n$ from $n = 2$ to $n = 4$. For the quantum-well state with $n = 1$, the dispersion is significantly less than that of the other quantum well states and corresponding calculated bulk value. We note that the deeper quantum-well states overlap the bulk bands in the substrate and so are really resonances; for such states the reflection phase shift at the interface is relatively slowly-varying and so the dispersions in Fig. 2 are approximately at constant $k_\perp$. In contrast, the energy of the $n = 1$ state is within the energy gap of the substrate, where the interface phase shift is rapidly varying. In this case, the dispersion in Fig. 2 includes an implicit variation in $k_\perp$ so that the curvature may not reflect the true effective mass. Further analysis of the dispersions and effective masses of quantum well states from different other coverages will be done.

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References: