Indication of Charge Density Wave Formation in Bi(111)

Christian R. Ast and Hartmut Höchst

Synchrotron Radiation Center, University of Wisconsin–Madison, Stoughton, WI 53589

The (111) surfaces of various face-centered cubic (fcc) metals (e.g. Al, Cu, Ag, Au) commonly show two-dimensional bands in the vicinity of the Γ-point. Their energy dispersion $E(k_x, k_y)$ follows that of a rotational paraboloid and their Fermi surface has circular shape. Recent photoemission studies found that Bismuth(111) shows a similar band near the Γ-point [1]. However, a detailed analysis of the FS reveals a hexagonal contour which is in contrast to the circular FS reported for other materials. These differences may be attributed to the highly anisotropic rhombohedral (A7) crystal structure of Bi consisting of bilayer planes perpendicular to the trigonal axis [2].

From temperature dependent measurements we found the onset of an energy gap at the Fermi level (FL). The presence of parallel sections in the FS combined with the observed energy gap provide necessary ingredients for the formation of an incommensurate charge density wave (CDW). To further support the CDW formation we have carried out model calculations of the Lindhard susceptibility based on mean-field theory in multiple dimensions.

FIG. 1: The Lindhard susceptibility of a hexagonal FS ($\chi^{\text{hex}}$) is compared to the 1D ($\chi^{\text{1D}}$) and 2D ($\chi^{\text{2D}}$) free electron case. The top left corner shows the direction of q with respect to the hexagonal FS.
Photoemission spectroscopy of Bi(111) reveals a small hexagonal two-dimensional Fermi surface (FS) associated with an electron band centered in the surface Brillouin zone. Along the hexagon the Fermi momentum $k_F$ ranges from 0.053 Å$^{-1}$ to 0.061 Å$^{-1}$. Temperature dependent valence band spectra show an anisotropic energy gap $\Delta$ near the Fermi level. At 70 K the gap ranges from 14 to 22 meV. Arguments based on susceptibility $\chi(\vec{q})$ calculations of a hexagonal FS are used to discuss a incommensurate charge density wave (CDW) formation associated with a $q_{CDW} = 0.106$ Å$^{-1}$.
