Quantum-well states affected by monolayer spacer in metal films

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Quantum-well states can be realized in a thin metal film, which confines the motion of the electrons in the direction normal to the film. There is spatial variation of the quantum-well wave function within a thin copper film, and a monolayer of magnetic material could effect the spatial variation. We employs photoemission experiments and first principles calculations to investigate the behavior of QWS when a monolayer of Ni or Co inserting the thin Cu film.

Motivation: QWS could modulated many physical quantities to exhibit oscillatory behaviors, so modulating QWS is very important . Make clear that how the QWS behave when modulated by different materials is helpful to design new generation electronic apparatus.

Quantum Well States in Co(100)/Cu(100) systems

There is a symmetry gaps in Co/Cu(100) systems, it can serve as potential energy barriers to confine electrons moving along these directions, leading QWS.

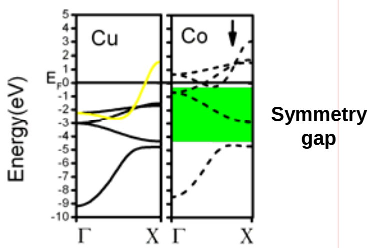

FIG. 1. bands of bulk Cu and Co

Those sp band QWS is local in the energy windows about 0~-2.0eV, could be explained by PAM mode excellently.

Phase accumulation model:

$$2(k_{BZ}-k)d-\phi_B-\phi_C=2\pi\nu$$

v= N-n ,N is the layer num of Cu, v is number of nodes of QWS.

QWS energy calculated using DFT:

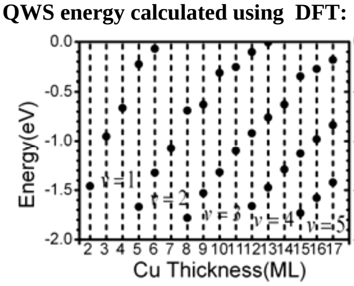

FIG. 2. QWS energy at surface Brillion zone center Γ

Fig. 3 show charge density of QWS(N = 9),enlevop wave-function is displayed.

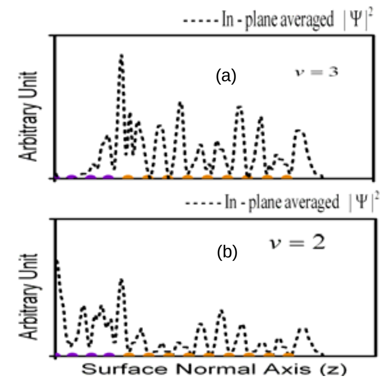

FIG. 3. In plane average charge density of QSW

A mono-layer of magnetic material interrupts QWS: difference between Co and Ni

Combining this with the use of two wedge-shaped samples (Fig. 4a), it is possible to investigate a monolayer Ni or Co inserting in different position of the QW[1,2] .

The FIG .4b is the pattern of photoemission spectroscopy of the sample in (a) which is inserted by a monolayer Co or Ni.

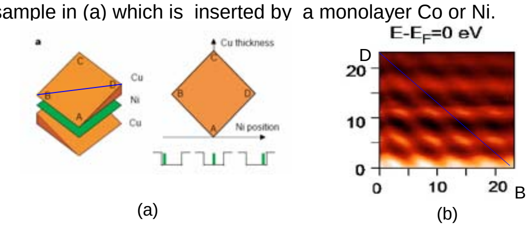

FIG. 4. Along line BD, the thickness of total width of QW is constant, but the position of monolayer magnetic material is change

	the photoemission intensity along BD
Co Spacer:	
At Fermi level:	oscillatory
Below Fermi level:	oscillatory
Ni Spacer:	
At Fermi level:	no oscillatory
Below Fermi level:	oscillatory

Band energy calculated using DFT when inserting a spacer in Cu

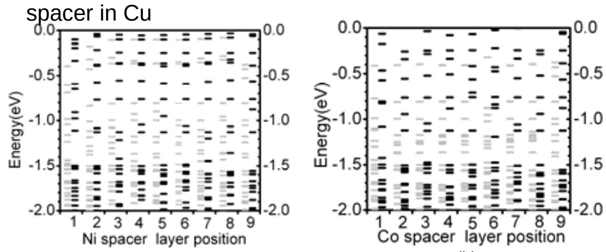

FIG. 5. The energy level of Γ point of 9 layers Cu thin films, with which a spacer layer shifts form the top to the bottom of it

There are four types of states in the energy window (0~-2.0eV): surface states, Co d-bands, Cu d-bands QSW(its energy all below -1.5eV),sp band QSW. What we interest is sp band QSW, which is select to display in the graph below.

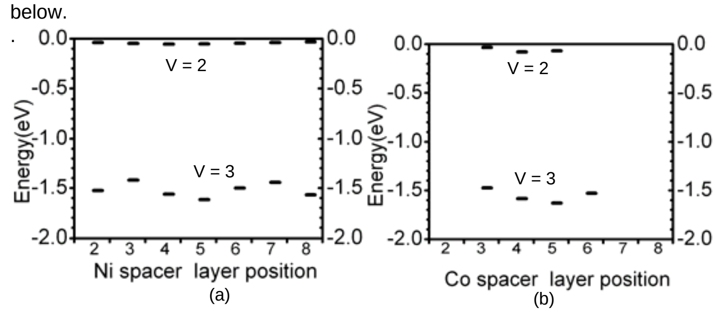

FIG. 6. The QSW energy level of Γ point of 9 layers Cu thin films, with which a spacer layer shifts form the top to the bottom of it.

The energy of QWS at Fermi level is has few oscillatory when inserting Ni as spacer. But when inserting Co at some position in Cu, the QSW at Fermi level disappear. Below the Fermi level, the QWS of both case have oscillatory, but only inserting Co will let some QSW disappear.

The In-plane average electron charge densities of FIG. 7 could be seen as evolutes from FIG. 3b.

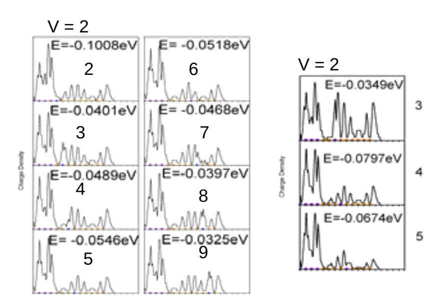

FIG. 7. In-plane average electron charge densities along the slab direction of QWS at Γ when inserting a spacer in Cu

Conclusion: From photoemission experiments and first principles calculations, we could confirm that at Fermi level there are different role between Co and Ni as spacer to modulate QSW. When inserting a Co spacer, there is oscillatory behavior for QSW at Fermi level, but no such oscillatory when substitute spacer as Ni. In all, Ni as a spacer has weaker effect than that of Co.

Reference: [1] Y. Z. Wu ect. PRB 73 125333 (2006) [2] R. K. Kawakami ect. Nature 398 132(1999)