

Electronic excitations in thin metallic films

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Confinement of valence electrons in metallic films of thickness comparable with the electron Fermi wavelength results in discrete quantum well states, which are the origin of quantum size effects in the properties of the system. Most theoretical studies have focused on the electronic structure of these systems and less attention has been paid to study of the electronic excitations.

At the same time, investigation of how the collective and single-particle electronic excitations evolve with the change of the film thickness present interesting problem, especially at the range of film thicknesses a few atomic layers. Recently this was investigated within framework of a jellium model [1]. In particular, there was demonstrated how size effects, i.e. discrete electronic spectrum in the direction perpendicular to the film surface influences excitations spectra. In present contribution we perform investigation of the evolution of the electronic excitations in thin Ag(111) films as a function of thickness considering its electronic band structure on a more realistic basis in comparison with the jellium model. For this we employ a model potential proposed in Ref. [2]. This potential mimics the atomic structure of the Ag(111) in the direction z perpendicular to the surface, and correctly reproduces the experimental Ag(111) work function, the projected bulk band structure, the surface and first image-potential states. With the use of this model potential we have performed self-consistent calculations of the surface response function of the Ag slabs of 1-10 monolayer thickness. For comparison, we also performed similar calculations using the energy band structure obtained within a conventional jellium model. The comparison of these two sets of data reveals striking differences in the excitation spectra of Ag films. The origin of these differences resides in the different band structures of two models. As an example, in Fig. 1 we demonstrate differences in the band structure for 4 ML slabs obtained in the two models. Thus, even for very thin films, in the case of 1D model potential one can observe two states (whose wave functions are mainly localized in vicinity of the surface atomic layers) with energies close to the Fermi energy (surface states) whereas the jellium model does not allow appearance of this kind of states. These differences in band structures are translated to the excitation spectra of these two models. As an example, in Figs. 2 and 3 we present excitation spectra for the 4 ML slab for the jellium and model potentials, respectively. The most pronounced differences correspond to interband transitions. A dispersive peak around 1eV in Fig. 3 corresponds to transitions between the partially occupied even and the empty odd surface states. An intraband region is qualitatively similar in both models. In this region the sharp linearly dispersing peaks correspond to Acoustic Surface Plasmon (ASP) [3]. Small differences in their dispersion are dictated by the band structure (at the $q=0$ point) and different effective masses which influence the Fermi velocities. For example, in Fig.1 the deepest occupied states have almost the same energies and effective masses which cause the similarity in the higher energy ASP branches in two models. On the other hand, for the higher occupied model potential states the effective masses are smaller unity that produces differences between the lower-energy ASP branches.

Note that upon increase of the slab thickness all the quantum size effects in the excitation spectra gradually vanish in the two models. However, the acoustic surface plasmon related to the Ag(111) surface state survives as was demonstrated previously [4].

References:

- [1] L. Marusic, V. Despoja, M. Sunjic, J. Phys.: Condens. Matter, **18** (2006) 4253.
- [2] E.V. Chulkov, V.M. Silkin, P.M. Echenique, Surf. Sci., **437** (1999) 330.
- [3] V.M. Silkin, A. Garcia-Lekue, J.M. Pitarke, E.V. Chulkov, E. Zaremba, P.M. Echenique, Europhys. Lett., **66** (2004) 260.
- [4] V.M. Silkin, J.M. Pitarke, E.V. Chulkov, P.M. Echenique, Phys. Rev. B, **72** (2005) 115435.

Figures :

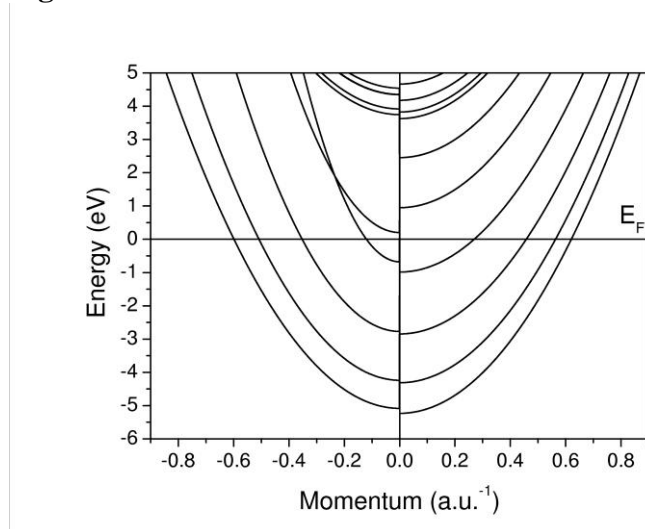


Fig. 1. Normalized Left side: Band structure for the 4ML Ag(111) film calculated by using the model potential of Ref. [1]. Effective masses from bottom to top are $m^*=0.96, 0.83, 0.61, 0.29, 0.44, 1.0, 1.0, 1.0, 1.0$. Right side: Band structure for the 4ML thick Ag film calculated by using the jellium model. Effective masses for all the bands are set to unity.

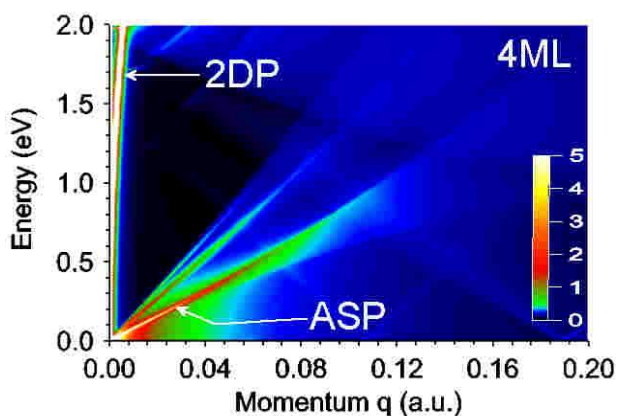


Fig. 2. Normalized surface loss function, $\text{Im}[g(q,\omega)]/q\omega$, for the 4ML thick Ag film calculated by using the jellium model.

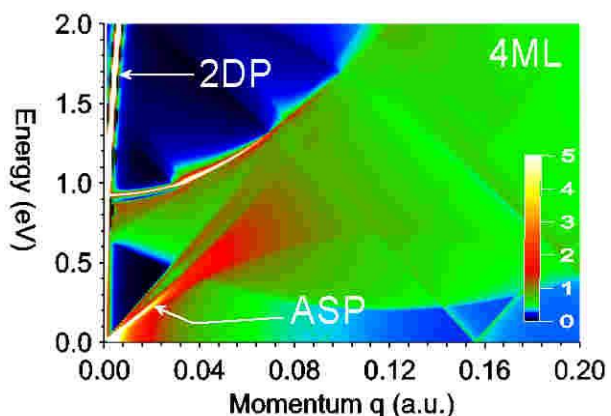


Fig. 3. Normalized surface loss function, $\text{Im}[g(q,\omega)]/q\omega$, for the 4ML thick Ag film calculated by using the model model.