CHARGE-DENSITY RESPONSE TO A STATIC IMPURITY AT Cu(111) AND Ag(111) SURFACES

V. M. Silkin[1], I. A. Nechaev[1], E. V. Chulkov[1,2], and P. M. Echenique[1,2]

[1]*Donostia International Physics Center (DIPC), P. de Manuel Lardizabal, 4, 20018 San Sebastián, Basque Country, Spain*
[2]*Departamento de Física de Materiales, Facultad de Ciencias Químicas, UPV/EHU and Centro Mixto CSIC-UPV/EHU, Apdo.1072, 20080 San Sebastián, Basque Country, Spain*
waxslavs@sc.ehu.es

Electrons occupying partly occupied s,p_z-surface states on closed-packed surfaces of noble metals form a two-dimensional (2D) nearly free electron gas. The scattering of these electrons off any surface imperfection such as steps, point defects and adsorbates produces oscillations in the electron density, which can be observed nowdays by scanning tunneling microscopy [1,2]. It has beed demonstrated that the period of these iscillations is determined by the surface state Fermi vector and its decay is well desctibed by the $1/R^2$ law predicted for a 2D electron system, R being a distance from the impurity along the surface [3]. However, in contrast to the pure 2D electron system, the surface-state wave function penetrates into the solid at a scale of few nanometers. Thus, the surface-state electron system coexists with underlying three-dimensional (3D) continuum which screens the external impurity by building up Friedel oscillations whose amplitude should fall off with the distance as . Recently, the question of how these both 2D and 3D electron systems respond simultaneously to an external impurity has been addressed in Ref. [4]. It has been demonstrated that the resulting induced charge-density behavior is more complicated than it follows from the previous theoretical studies. Two main observations have been made. First, the decay inherent to the 2D electron systems is also observed in the 3D electron system in the vicinity of the surface. Second, in comparison with the jellium model, the significant modification of the charge-density oscillations decay far into the interior of the solid has been found. In the present contribution we examine these two points in attempt to understand its origin. For this we analze the induced charge-density produced by an external charge at the Cu(111) and Ag(111) surfaces.

Our approach is based on linear response theory which relates external perturbation and the corresponding induced charge density through the equation

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where is the density response function which satisfies an integral equation

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with being the Coulomb potential and the response function for a noninteracting electron system. χ^o contains information on all electronic transitions in the system, both

intraband ones within 2D and 3D and interband ones between 2D and 3D [4].

In this contribution we present the calculated induced density as a function of and for an impurity placed at the crystal edge. We find that the behavour of induced density for Cu(111) and Ag(111) is very similar, whereas it is very different from that obtained for jellium model. We observe a chess-board-like pattern in the induced density close to the surface and its deep penetration inside the solid with the angle to the surface normal. To clarify the origin of these two observations we have performed calculations of the induced density with and without the inclusion of electron transitions in χ^o from both 2D and 3D electron systems. Analising the results obtained we conclude that the combined response of the 2D electron system to the external impurity and the 3D electron system to the electrostatic field created by the charge-density induced in the 2D system by this impurity is responsible for the appearance of the chess-board-like pattern in the vicinity of surface. As for the penetration of the charge-density into the solid at finite angle, this effect is completely defined by the 3D system response. From the comparison results for Cu(111) and Ag(111) we have found that the penetration inside the solid depends on both the impurity position and the projected bulk electronic structure.

References

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