Theoretical Studies of Ultrafast Processes at Metal Surfaces

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Abstract: Some theoretical models of the process occurring in infrared laser assisted photoemission from the metal surfaces and photoionization of adsorbated on such surfaces atoms by the attosecond pulses will be discussed. The development of such methods is urgent for understanding of the experimental findings.

The sub-femtosecond pulse technique [1] has its aim to study superfast relaxation processes caused by an abrupt change in the electron subsystem after an electron ejection. Application of this technique to solids is of great interest because a vast number of transient electron phenomena at surfaces and in solids does evolve on a few femtosecond - subfemtosecond time scale. Although the dynamics of electrons in condensed-matter systems is very complicated, its comprehensive theoretical understanding is necessary for promoting experimental investigations and their application in nanotechnology.

The first experimental study of this dynamics was performed in Garching [2] and the computational simulation of the experimental findings was presented in [3]. The computations nicely reproduced the observed effect. The important ingredients of the theoretical model are the assumptions that the strong infrared laser field is promptly screened in the metal and that the electrons in the metals have a rather short mean free path.

For the investigations of the fast processes at the metal surface it seems very perspective to use, as a mechanism for abrupt change of the external charge, the ionization of an adsorbate by attosecond pulse. A basic computer code is developed [4] for simulation of the infrared laser assisted ionization of an adsorbate by attosecond pulse. In the code, the interactions of the ejected electron with the adsorbate core, its electrostatic image, the metal bulk, the infrared laser pulse, and the attosecond extreme ultraviolet pulse are taken into account. The interacttion between the ejected electron and its electrostatic image is taken within the simplest conventional approximation. This code and some results obtained with its implementation will be presented in the talk. The code is rather versatile and its possible development will be discussed.

In the processes with metal surfaces, the first feature to be discussed is formation of the response charge density in the metal and its influence on the ejected electron motion. In the text books the interaction between a charged particle with the electric charge q and a conducting plane surface is described by the potential energy $-q^2 / 4z$, where z is the particle coordinate perpendicular to the surface ($z = 0$ at the metal image plane, z is positive to vacuum). This potential energy has been obtained within the classical electrodynamics with the assumption of infinitely slow motion of the charged particle from infinity to the surface, so that the electron system of the metal follows this motion adiabatically. However, when an atom adsorbed on a metal surface is ionized, the ejected electron does not move slowly. This means the conventional theory of the ejected electron - metal surface interaction must be revisited. At first stage of the process, just after the electron ejection at the point z_0, the electron moves fast in the field of the adsorbate core, while the induced in the metal charge distribution remains almost frozen. At this stage, the attraction of the electron by the induced charge distribution is greater than it is within the adiabatic treatment. Then, the initial image charge decays (oscillating with the surface plasmon frequency), while the field due to the dynamical screening of moving electron arises (also with oscillations). A theoretical self-consistent consideration of motion of an electron ejected from an alkali atom adsorbed on a metal surface will be presented in the talk. It is shown that the dynamical effect leads to a decrease of the ejected electron energy by about 1-2 eV [5].

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