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Work function for the deformed metal surface

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Abstract

A method of calculation of work function for strained real metal surface is suggested. The method is based on connection between work function and the atomic electro-negativity and takes into consideration formation of the surface nanometer defects. The presented results of calculations for aluminum and copper are in good accord with the experimental data.

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1. Introduction

Work function (WF) of metals has been studied experimentally under various conditions of strained state [1,2]. It was found that elastic strain increases WF up to several meV. WF of the plastic deformed metals decreases by tens and hundreds meV.

In this paper [3] a stabilized jellium model within the self-consistent Kohn–Sham calculation method is considered; stabilization energy and consequently work function, surface energy, etc. as functions of electron density and deformation

are derived. However, a physical model, which would be able to explain changes of WF for surfaces with crystals defects, has not been worked out as yet. Calculations of WF for real metal surfaces based on quantum mechanics are too complicated.

The authors [4,5] have proposed a method of WF calculations for a non-ideal surface. This method is based on the semi-empirical theory of the neutral orbital electro-negativity (NOE). The general idea is that work function can be represented as the orbital electro-negativity localized close to atom on the surface. The surface constituent of WF is changed with strain considerably as the surface potential changes abruptly. In their turn these changes depend upon the surface microgeometry and upon the coordination of

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atoms on it. The determination of the surface atomic coordination has become possible due to the last achievements in the scanning tunnel microscopy [6,7].

The ground for the work was the fact that till today there is no calculation scheme for determining work function (WF) of real metallic surfaces. The quantum mechanics methods solve the problems for metal surfaces with regular structure [8,9] and with indirect deformation consideration [10]. The proposed scheme of calculation does not worse other semiempirical methods [11]. At the same time, it has some advantages. Due to the experimental data of scanning tunneling electron microscopy, information about nanometric geometry of surface at metal's deformation can be obtained [7], and it is possible to calculate WF of any surface unit in accordance with the known atom distribution over the surface.

The aim of this work is to develop the method of WF calculation for the strained real metal surface. Connection between work function and atomic electro-negativity taking into consideration formation of surface defects is used in this work.

2. Physical model

The numbers of disrupted interatomic bonds with the nearest and with the distant neighbors, i, j , respectively, are used for the characteristic of the surface imperfection. Dependence of WF on i and j may be expressed as [4]

$$\begin{aligned}\Phi_{ij} &= x_{ij} \\ &= 0.98 \frac{(V_n - i)n_a + (V_{nn} - j)n_b + 1}{r_a} \\ &\quad + 1.57 \text{ eV},\end{aligned}\quad (1)$$

where x_{ij} is the orbital electro-negativity of an external atom on the surface; V_n and V_{nn} are numbers of the nearest and the next neighbors of atoms in volume, respectively; these numbers are dependent upon the type of crystal lattice; $(V_n - i)$ and $(V_{nn} - j)$ are the numbers of bonds of the external atom with the nearest and the next neighbors; n_a and n_b are the numbers of electrons taking part in bond of the surface atom with the nearest and

the distant neighbors, referred to one atom; r_a , Å, is the atomic radius of the element according to Pauling. The formula (1) is semiempirical; the detailed substantiation of the constants is in the article [12]. In the formula (1) x_{ij} , it is identified with potential Z^*e/r_a on covalent border of atom radius r_a , Z^* —the effective charge of a nucleus influencing on electrons of valence orbital. Dependence x_{ij} from number of valence electrons in (1) is determined by mutual screening of valence electrons (effective screening constant equals 0.5). Coefficients 0.98 and 1.57 are determined by adjustable parameters.

Formula (1) well describes the experimental data on work function of monocrystal planes of metals. Calculations of WF of some metals were executed on the basis of the theory of neutral orbital electro-negativity. The results of these calculations are in accord with the experimental data. It is shown in Fig. 1, constructed on the basis of the data taken from the work [13].

WF of the non-ideal surface of metal can be considered as the average value of electro-negativity of external atoms of metal. On close-packed monocrystal metal surface all external atoms are identical, therefore their total contribution is identical too in any point outside the surface. Close to

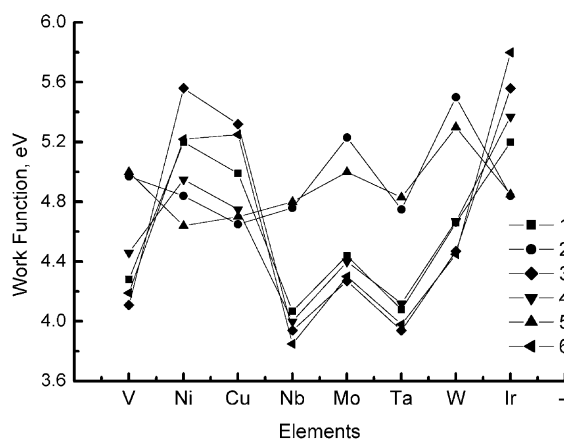


Fig. 1. Values of work function of electrons for monocrystals of different elements. Calculation by the method of neutral orbital electro-negativity for planes 1: (100); 2: (110); 3: (111). Experiment (the method of contact potential difference (CPD)) or the method of thermo-ionic emission (TE) for planes 4: (100); 5: (110); 6: (111).

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