

ON THE WORK FUNCTION  
AND SCHOTTKY BARRIER HEIGHTS OF METAL  
NANOFILMS IN A DIELECTRIC ENVIRONMENT

*A. V. Babich*

Zaporizhzhya National Technical University  
(64, Zhukovskii Str., Zaporizhzhya 60063, Ukraine;  
e-mail: [andrei\\_babich@mail.ru](mailto:andrei_babich@mail.ru))

S u m m a r y

We suggest a method for self-consistent calculations of the characteristics of metal films in a dielectric environment. Within a modified Kohn–Sham method and the stabilized jellium model, the most interesting case of asymmetric metal-dielectric sandwiches is considered, for which the dielectric media are different on the two sides of the film. We calculate the spectrum, electron work function, and surface energy of polycrystalline and crystalline films of Na, Al, and Pb placed into passive isolators. It is found that a dielectric environment generally leads to a decrease of both the electron work function and the surface energy. It is revealed that the change of the work function is determined only by the average of dielectric constants on both sides of the film. We introduced the position of a conduction band in the dielectric as a parameter in the self-consistency procedure. The calculations with the use of the image potential for an aluminum film with ideal interfaces vacuum/Al(111)/SiO<sub>2</sub> and vacuum/Al(111)/Al<sub>2</sub>O<sub>3</sub> and the sandwich SiO<sub>2</sub>/Al(111)/Al<sub>2</sub>O<sub>3</sub> are performed. As a result, the effective potential profiles and the Schottky barrier heights are calculated.