MODELLING THE ELECTROCHEMICAL AND CATALYTIC PROCESSES ON METALS ALLOYS AND SEMICONDUCTORS: LASER RADIATION EFFECT

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Paper is devoted to quantitative studying the laser radiation effect on electrochemical and catalytic processes on metal alloys and semiconductors in order to carry out the theoretical basis's of the corresponding sensors. The attempts of quantitative description of the metals (alloys) electron structure in the electrochemical processes, which take place, for example, on electrodes of the electrochemical generators have been undertaken in a whole number of papers (c.f.[l]), f.e. with the use of density functional theory. In these quite effective from calculations point of view models a description is produced on the language of the electron density on the metal surface. As result, these models are not enough sensitive to value and states density on the Fermi surface. Naturally there is a great number of papers (c.f.[3]) with using ab initio quantum chemistry methods. Such calculations give useful information, but some important moments of physical-chemical nature of the processes often remain in known degree veiled. As alternative one could consider the effective approaches, based on the electrodynamics and quantum chemical models [1-5]. Here we develop a new approach to laser radiation effect on electrochemical & catalytic processes on the metals, binary metallic alloys, semiconductors) and predict a number of new photo effects of the drastic influence of the laser radiation on characteristics of the cited processes [6]. A key moment is in adequate choice of the effective potential field of materials medium and obtaining a direct link between electron structure parameters of materials, electrochemical properties and laser radiation parameters with further numeral solution of equations of the Kohn-Sham type and the bound states type analysis. Simple electron gas and Thomas-Fermi approximations have been checked [1,2]. There have been found the electron structure parameters of the metal alloys, semiconductors, which define catalytic activity of materials to the simple model reactions of the following type: $H=H^{+}+e^{-}$, $O_2+e=0_2^{-}$. It is quantitatively shown how the Fermi level position dependence on the metal alloys components concentration influences on the electrochemical and catalytic properties. It is shown that the laser radiation effect allows to influence drastically on the studied processes. Quantitative results are obtained for different materials (transition metal alloys, Si,Ge semiconductors, lanthanide's perovskites).

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