A DFT study of the influence of a cathode surface state on its dark current emission.

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Under high electric field and in ultrahigh vacuum (UHV), electronic emission from a cathode leads to a low intensity current which is a field emission type one often called dark current[1]. While such field emission may be sought purposely, it can also be a serious problem, notably in the context of the neutral beam injector systems of the future nuclear fusion power prototypes[2] (ITER and DEMO) for which long-term maintenance-free injector operations remain highly challenging[3].

One well-known method of reducing the intensity of this detrimental dark current is by raising the gas pressure in the UHV cavity[4]. There is however no consensus in the literature on the mechanism leading to this current reduction[1] and thus on how to achieve it in a controlled way in engineering applications. We propose in the present contribution a model which relates the current intensity changes to modifications in the structure of the emitting surface, following gas injection. More specifically, we show how the presence of the gas modifies the carbon adlayer which covers the emitting cathode and thus influences the dark current intensity. Indeed, it is well known that current intensity is related to the work function of the cathode[5]. Using periodic Density Functional Theory, we study the effect of the carbon adlayer on the work function and on the emitting properties of the tungsten or the tungsten carbide (WC) cathodes used in the experiments[1]. The presence of a strong surface electric dipole due to the large electronegativity difference between carbon and metal induces important modifications in the work functions. We discuss, between the chemical nature and the morphology of the adlayer, which is the most influent factor on the dark current intensity. As a side issue, we also study the structure of the carbon adlayer as a function of its thickness and analyze possible formation of *graphene* physisorbed on the cathode.

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