Role of electron tunneling in the thermalization of the adsorbate at solid surfaces

Pawel Strąk¹, Pawel Kempisty¹, Konrad Sakowski^{1,2,3}, and Stanisław Krukowski¹

¹ Institute of High Pressure Physics, Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

² Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, ul. Banacha 2, 02-097 Warsaw, Poland

³ Research Institute for Applied Mechanics, Kyushu University, Kasuga, Fukuoka 816-8580, Japan

A new type of the thermalization processes of the adsorbates at solid surfaces are devised and presented. The scenario is based on an existence of the electric dipole layer at the solid surfaces. This field arises because the electron wavefunctions extend beyond the positive ions plane, denoting the microscopic location of the surface, thus creating strong local electric field, which drags the electrons into the solid interior and repels the positive ions. During adsorption of any molecular or atomic species at the surfaces of the solids, this field enforces the electrons tunneling into the solid interior. In the tunneling process, the electrons are drastically accelerated acquiring high kinetic energy, which is transported by the same electrons into the depth of the crystals. At the same time, the electron stripping of the adsorbates creates positively charged ions (atoms or molecules) which are retarded by the field, loosing most of the excess kinetic energy. In the result, they are landed smoothly at the surface and positioned in the adsorption sites. According to the scheme, the excess kinetic energy is not dissipated locally thus avoiding local melting of the lattice or creation of defects at the impact site. That explains the absence of kinetic surface damage, which is in accordance with the experiments. The scenario is supported by the *ab intio* calculation results, including density function theory of the slabs representing AlN surface and the Schrodinger equation for time evolution of hydrogen-like atom at the solid surface [1,2].

[1] P. Strak, P. Kempisty, K. Sakowski, S. Krukowski, Phys. Chem. Chem. Phys. 19 (2017) 9149

[2] P. Strak, P. Kempisty, K. Sakowski, S. Krukowski, J. Phys. Astron. 5 (2017) 4