Title: Computer simulations of characteristics of metal desorption from the Si(111) surface

Author: Adam Sikora

Department: Department of Surface and Plasma Science

Supervisor: RNDr. Pavel Kocán, Ph.D.

Abstract: In case of desorption of some metals (Pb, In, Ga) from surfaces Si(111) and Ga(111) was by use of integral techniques surprisingly observed zero-order of desorption. Theoretical explanation of zero-order is still missing, since it appears that the conditions that normally lead to desorption of the zeroth order - high diffusivity, the existence of 2D gaseous phase etc. - can not be met. The aim of this work is to develop kinetic Monte Carlo computer code for simulations of atomic processes on the surface of Si(111). The developed code will then be used for investigation of desorption spectra for various parameters and also for finding the parameters which allow the zero-order desorption.

Keywords: Kinetic Monte Carlo, temperature programmed desorption, zero-order desorption, Si(111)