THE ADSORPTION KINETICS OF HYDROGEN-LIKE PARTICLES IN POROUS Si

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S u m m a r y

We have modeled the processes of adsorption of hydrogen-like particles in porous silicon at the initial time moment of the physical adsorption. A model of cylindrical pores in Si is developed with regard for hydrogen admixtures. We have calculated the potential energy of interaction of drifting particles with the wall of a pore and determined the parameters of the adsorption centers. The simulation algorithm which is based on the methods of molecular dynamics and accounts the phenomena of diffusion, drift, adsorption, and desorption is proposed, and the distributions of the concentrations of adsorbed particles at various pressures and temperatures are obtained.