

DIFFUSION OF OXYGEN  
ATOM INTO SUBSURFACE  
LAYERS OF  $\text{Ge}_x\text{Si}_{1-x}/\text{Si}(001)$  INTERFACE

*T.V. Afanasieva, A.A. Greenchuck, I.P. Koval',  
M.G. Nakhodkin*

Taras Shevchenko National University of Kyiv  
(64, Volodymyrs'ka Str., Kyiv 01601, Ukraine;  
e-mail: greenchuckaa@gmail.com)

S u m m a r y

*Ab initio* calculations have been carried out to verify a possibility for an oxygen atom to transit from the bridge bond between the addimer atoms and atoms in the second subsurface layer to the bond between atoms belonging to the second and third subsurface layers of the  $\text{Ge}_x\text{Si}_{1-x}/\text{Si}(001)$  interface in the cases where one to three oxygen atoms are adsorbed. Such a transition was found to be unfavorable in the case where pure, Si–Si, and mixed, Si–Ge, addimers are present at the  $\text{Ge}_x\text{Si}_{1-x}/\text{Si}(001)$  interface. If only pure Ge–Ge addimers are present at this interface, the diffusion of a single oxygen atom is possible, with the corresponding diffusion barrier being 2.09 eV. Pure Ge–Ge addimers at the  $\text{Ge}_x\text{Si}_{1-x}/\text{Si}(001)$  interface favor the oxygen diffusion into the bulk to a greater extent than pure Si–Si and mixed Si–Ge addimers do.