Halogen Adsorption on III-V Semiconductor (001) Surface

Svetlana Kulkova[1,2], Aleksander Bakulin[2], Sergey Eremeev[1,2], Oleg Tereshchenko[3]

[1]Institute of Strength Physics and Materials Science SB RAS, Russia

[2]Tomsk State University, Russia

[3]Institute of Semiconductor Physics, Novosibirsk, Russia

e-mail: kulkova@ms.tsc.ru

For modern technology it is very important to develop techniques such as layer by layer removal of a semiconductor, keeping well-ordered, atomically flat and stoichiometric semiconductor surface. Since III-V semiconductors (001) surface represents alternating layers of anion and cation, these semiconductors are ideal candidate for making such atomically abrupt structures. Digital etching of III-V semiconductors can be realized by means surface reactions with adsorbates interacting selectively with atoms of group III or group V.

We present comparative *ab-initio* study of the halogens (F, Cl, I) adsorption on the cation-rich GaAs and InAs ζ–(001)-(4×2) surface as well as Cl adsorption on InAs β3′-(4×2) performed by means of the pseudopotential plane-wave method within density functional theory. The most preferable position for halogens were found above dimerized Ga (In) atoms in the case of ζ– (001)-(4×2) surface. As seen from Fig. 1 the accumulation of a large negative charge between cation dimer atom and halogen occurs upon adsorption at M_1 (the same trend takes place for M_2, M_3, S_1 sites also), whereas the charge depletion is observed between cation and anion surface atoms. The opposite trend occurs when halogen is adsorbed above As-trench edge atom (S_7) - the depletion of charge occurs in the region of halogen-As bond. Atomic and electronic structure of new β3′-InAs(001)-(4×2) reconstruction is discussed. It was show that independently on surface reconstruction, halogen prefers to bond with In dimerized atoms. In general, halogen interaction with semiconductor surface leads to the weakening of the chemical bonds between surface atoms that determines the initial stage of surface etching.

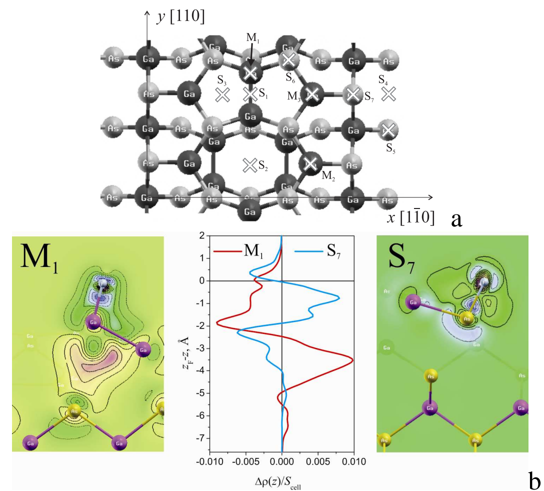

Fig. 1 Atomic structure of ζ-(001)-(4×2) surface and adsorbate sites (a). Charge density difference $\Delta\rho(r) = \rho_{Ga(In)As}(r) + \rho_{Halogen}(r) - \rho_{Halogen/Ga(In)As}(r)$ for M_1 and S_7 fluorine adsorption sites and integrated Δρ in the direction parallel to surface as a function of Z into the bulk (b).