For pSi-n$(Si_2)_{1-x}(CdS)_x$ structures (fig.2,a) the maximum of the photo-response before irradiation is observed at the photon energy $E_{h\nu} \approx 1.7$ eV, and after irradiation at $E_{h\nu} \approx 1.88$ eV. Depth of p-n junction is ≈ 10 microns. The part of electron-hole pairs photogenerated by high energy photon in the layer near the surface does not reach the dividing barrier that results to decrease of photoresponse in short wave part of spectrum. Hence, in epitaxy layers the diffusion length of minority carriers is less than 10 microns. Increase of the spectral sensitivity after irradiation for pSi-n$(Si_2)_{1-x}(CdS)_x$ as well as for pSi-n$(Si_2)_{1-x}(ZnSe)_x$ structures, apparently, is caused by increasing of life time (τ_p) and mobility (μ_p) of minority carriers that results in increase of diffusion length of minority carriers - $L_p = m_p t_p kT/q$. After the irradiation of pSi-n$(Si_2)_{1-x}(ZnSe)_x$ structures at dose 10^4 rad and pSi-n$(Si_2)_{1-x}(CdS)_x$ structures at 10^5 rad the photo-response spectrum (fig.2a,b) obviously shows the photosensitivity peak at photon energies $E_{h\nu} \approx 2.54$ eV and $E_{h\nu} \approx 2.4$ eV, accordingly. These peaks are caused by admixtures of ZnSe or CdS which form impurity levels in the valence zone of silicon. Increase of constant relaxation time and photosensitivity in short-wave part of spectrum, apparently, is caused by radiation-stimulated solid phase effects of small doses of γ-irradiation.

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STABILIZATION OF HOLLOW SPHERICAL SILICON NANOSTRUCTURES PREDICTED BY NON-CONVENTIONAL TIGHT BINDING METHOD

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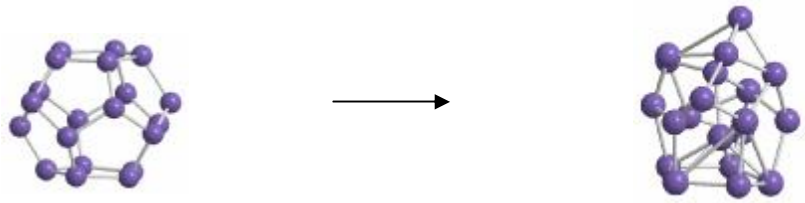
Discovery of the carbon hollow nanoclusters, which have pentagons and hexagons on their surface (fullerenes), has led to interest in the possible existence similar structures for the other elements, particularly silicon. In the present work the possibility of the stabilization of the fullerene-like hollow silicon cluster containing 20 atoms has been investigated computationally, using the non-conventional tight binding method [1].

Simulation of the hollow spherical 20-atomic silicon nanostructure with pentagons on the surface has shown that energy minimization takes the cluster from its original hollow fullerene-like shape to an asymmetric elongated compact form. This structure has primarily rhombic figures on its surface and a 4-atom chain inside. Coordination numbers of atoms in this structure are increased relative to the initial structure. The final structure obtained is similar to the quasi-one-dimensional pentagon-based Si_{19} cluster that we have reported earlier[1]. The cohesive

energy per atom for the quasi-one-dimensional Si_{19} cluster is favorable than for the Si_{20} (4.112 eV for Si_{19} and 3.698 eV for Si_{20}).

Si_{20} structure is shown on the picture below:



Initial hollow cage

The elongated compact form obtained after optimization

Two possible means of stabilizing the Si_{20} cage were considered: (1) surface saturation and (2) filling of the cluster internally with hydrogen atoms.

The first approach showed that the $Si_{20}H_{20}$ silicon cage saturated entirely by hydrogen atoms is the most stable structure with total cohesive energy of 250.4749 eV. The cohesive energy lowered (up to 127.1785 eV) upon decreasing the amount of hydrogen atoms on the cluster surface and distortions changed the structure to a more compact form. The HOMO-LUMO gap has a trend to widen from 0.08 eV for $Si_{20}H_{10}$ to 2.28 eV for $Si_{20}H_{20}$.

Filling the cage Si_{20} with H_2 molecules has been done step-by-step. The maximum amount of hydrogen molecules ***n*** was 10. The clusters were found to be unstable. The cage opened and hydrogen atoms escaped from the cluster for ***n*** = 3, though pentagons remained on the surface (as shown on the picture). In the case of $Si_{20}H_2$, a H_2 molecule broke and hydrogen atoms bonded to the silicon atom forming a bridge structure.

$Si_{20}H_2$ $Si_{20}H_6$

Thus, molecular dynamics simulation of the hollow spherical Si_{20} cluster has shown that filling the cluster internally with hydrogen atoms did not stabilize the silicon cage and led to distortion of the cluster, while a full externally saturation of the surface by hydrogen atoms resulted in a stable hollow cluster $Si_{20}H_{20}$.

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