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Program and Abstracts

Microstructure of the relaxed (001) Si surface

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We have applied molecular dynamics method and semi-empirical potential [1] to obtain the realistic picture of Si surface layers relaxation.

The starting configuration was taken as a parallelepiped containing 864 atoms. There were 12 layers with 72 atoms in each one. Periodic boundary conditions were used in two dimensions.

Investigation of full Si surface relaxation leads to structural defects and dangling bonds arising as it was shown in the case of amorphous Si modeling [2].

The result is that during relaxation a rebuilding and a re-hybridization of chemical bonds take place. Such procedure leads to arising of non-usual polygons with $n=3-9$ and nodes with $1-3$ electrons that do not participate in chemical bonds creation. Thus there are nodes with more than one dangling bond. Computer calculations allow obtain the radial distribution function (RDF) and the angle distribution function (ADF) (the angle between chemical bonds directions are implied).

The chief conclusion is that a quasi-disordered phase (QDP) arises as a result of free Si surface relaxation. The RDF and ADF are similar to those for a-Si. Each of upper four layers has his specific structural characteristics. The third layer is the most "perfect" one.

Only this layer in a surface QDP is without nodes that have two dangling bonds. But at the same time the third layer is the most distorted. Atoms of this layer are characterized by the largest displacement with reference to their normal position in the crystallographic plane. Thus the third layer in surface QDP plays a special transitional role between the crystal volume and the surface QDP.