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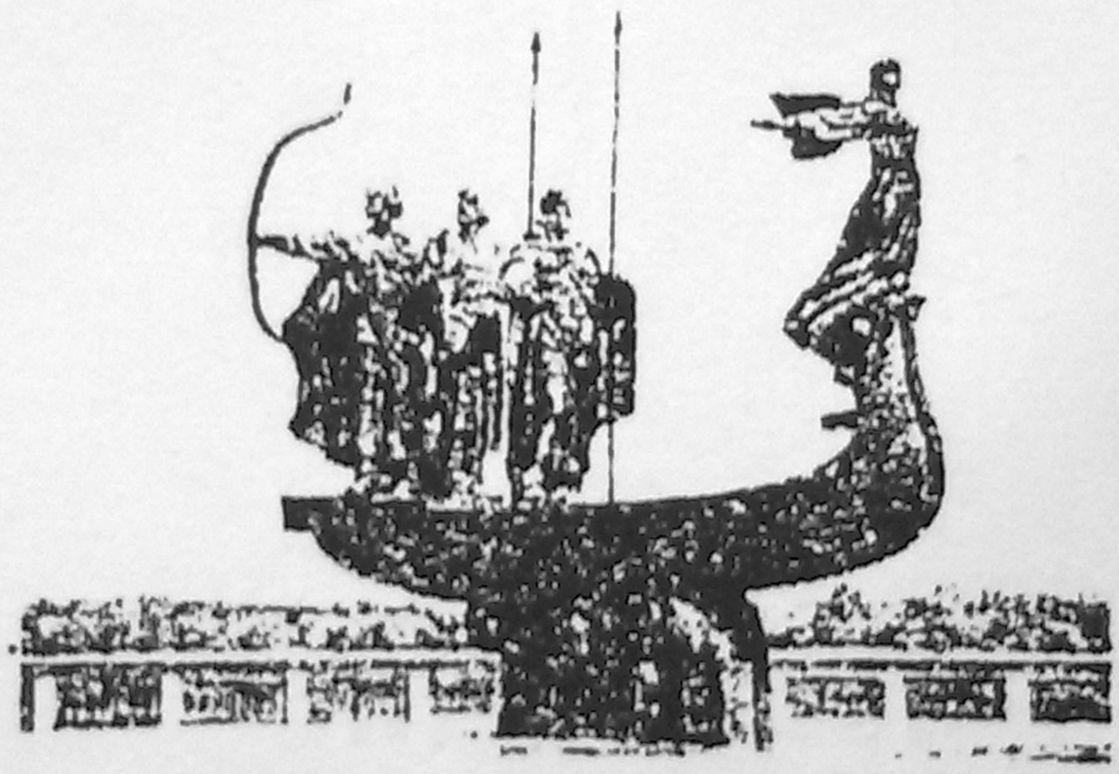

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Abstracts

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[Inv 7]

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.

At first all atoms were in normal lattice positions. The relaxation of Si surface, which corresponds to (001) plane was investigated. MD method was

applied in its standard form i.e. the equations of motion were solved by using of the central difference scheme. The time-step was 10-14s.

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].

A primary crystal had a given temperature and after "cutting" of a crystal we had a corresponding temperature of the crystal surface. Relaxation processes were observed at temperature 290 K.

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. This QDP has some peculiarities. Each of mentioned four layers have his specific structural characteristics. The third layer is the most "perfect" one. This layer has only 2,8% dangling bonds and what's more such nodes have only one non-paired electron (n (1) = 2,8%).

Besides, only the third 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.

1. F.H.Stillinger, T.A Weber, Phys. Rev., B31, 9262 (1985)
2. P.W.Jacobs, A.E.Kiv, R.M.Balabay et al., RAU Sci. Rep., Computer modeling & New Technologies, 2, 15, (1998)