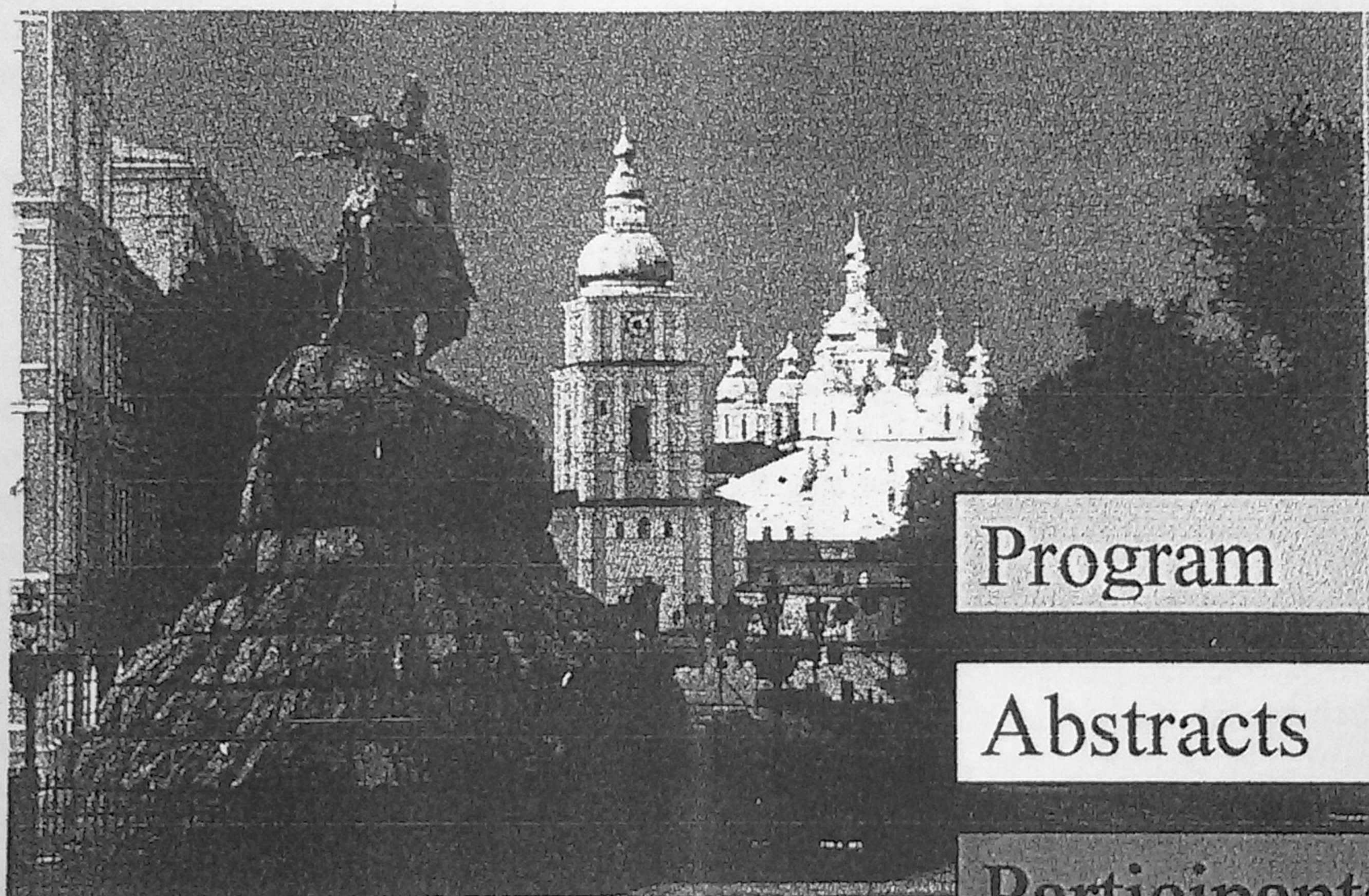


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MD Simulation of the Ion-Stimulated Relaxation in Silicon Surface Layers

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A widespread technological process in microelectronics is radiation treatment of silicon surface. The problem is to clarify conditions of the ion irradiation and to determine parameters of ion beams, which may stimulate relaxation processes leading to the best surface characteristics.

A Molecular Dynamics (MD) code was applied which is suitable to investigate both surface features and bulk properties of Silicon. A starting configuration was taken as a parallelepiped containing 864 atoms. Periodic boundary conditions were applied in two dimensions. Relaxation processes induced by ion bombardment were studied at the temperatures from 290 K to 1000 K. New algorithm was used which allows for each atom to change his neighboring atoms and create chemical bonds with new four nearest atoms. So the relaxation is accompanied by rebuilding of chemical bonds and their re-hybridization [1]. The results of computer simulation of Si surface relaxation processes have shown that at elevated temperatures a quasi-disordered phase (QDP) arises as a result of free relaxation of Silicon surface. The model has emphasized that in particular the microstructural constituents in QDP of Silicon surface layers are nodes with one or more dangling bonds.

Influence of bombardment of Silicon surface by low energy neutral particles on relaxation processes in near surface layers was studied for energies of bombarding particles in vicinity of the energy threshold E_d for elastic displacements: 10, 20, 30, 40 and 50 eV. In simulation procedure one impulse corresponded to $2 \cdot 10^{12}$ particles/ $\text{cm}^2 \cdot \text{s}$.

For monoenergetic monoisotopic ion bombardment the induced structural changes are depended on the bombardment angle. Therefore we have compared the results for different energies of ion beams at the same bombardment angles, ion doses and dose rates.

A specific energy dependence of radiation-stimulated relaxation processes was obtained. Just it was established that the ion irradiation of Silicon surface in vicinity of E_d leads to extreme values of structural characteristics of near surface layers. In particular, for parameter ΔE , which characterizes the level of relaxation and, and for parameter of the relaxation time the extreme energy dependences take place. The optimum energy in all cases lies in vicinity of E_d . Thus it was established that ion bombardment of silicon surface in the energy region of the threshold of elastic displacement of atoms might allow to improve structural characteristics of surface layers and to decrease the relaxation time. Energy dependencies of radiation induced processes show a possibility to improve the real structure of Silicon surface and to accelerate the long-term surface relaxation in microelectronic technology.

1. P.W. Jacobs, A.E. Kiv, R.M. Balabay et al. Computer Modeling & New Technologies (1998) Volume 2, pp.15-20