A Molecular Dynamics Study of Radiation Induced Electrostatic Disruption of Insulator Surfaces

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A molecular dynamics simulation is applied to study radiation induced electrostatic disruption of insulator surfaces such as polymers. The behavior of model is similar to a previously proposed ion explosion spike mechanism. Thermal equilibrium properties of the bulk insulators are studied in terms of equipartition of energy and thermal expansion. The static relaxation and cohesive energy of insulator surfaces are examined.

With the correct thermal equilibrium properties of insulator surfaces, we are able to study electrostatic disruption by using a scaled Lennard–Jones potential. The computational cell contains 600 atoms in a 2D surface and is first surrounded by a thermal conducting boundary, and next by a fixed boundary of atoms. This model includes interaction and energy flow between atoms in the cell and the bulk of the solid.

Electrostatic disruption is initiated by placing single positive charges on two to six neutral atoms in the surface region. Three stages have been identified in this disruption process. First, rapid ejection of several atoms (5 to 15) occurs at $\sim$ 0.5 ps, compared to the Debye period 0.1 ps. Secondly, many atoms in the vicinity of the charged region are greatly disturbed. Craterlike defects and voids are generated by the Coulomb explosion, and atoms are piled up at the surface. Thirdly, the temperature of the surface becomes higher than the background temperature, enhancing the sublimation and annealing of atoms in this region. For charges deposited deep inside the surface there are unusually large atomic displacements but no rapid ejected atoms. The effect of different initial thermal conditions has been studied, and the calculations show some fluctuations but no significant change in the overall results. As more charges are deposited near the surface, electrostatic disruption becomes more violent and leads to high ejection yields.