MOLECULAR DYNAMICS STUDY OF SURFACE NANOSTRUCTURE EVOLUTION BY Ar ION BOMBARDMENT

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High energy ion bombardment on solid surface has attracted much attention owing to its capability to fabricate ordered nanoscale structures such as self aligned quantum dots. We employed classical molecular dynamics (MD) simulation to investigate the details of the surface structure evolution during the high energy Ar bombardment on Au and Pd (001) surface. When Ar bombarded on the Pd surface with high incidence energy, the substrate atoms were not only eroded but also rearranged to locate higher than the initial surface in a ballistic manner. Quantitative analysis showed that the number of the rearranged atoms, defined by the atoms located higher than the initial surface, is as 3 times larger than that of the eroded atoms. Lateral distribution of the rearranged atoms was investigated in a statistical manner by summing up the distribution of the rearranged atoms for 1,500 independent bombardment events. The distribution of the rearranged Pd atoms reveals 4 fold symmetric pattern when the incidence angle ranged from 0 to 60 degree. Previous experimental result which showed 4 fold symmetric autocorrelation function of the surface [1] would be discussed in terms of the rearrangement pattern to reveal the significant role of the ballistic rearrangement of the substrate atoms in the nanoscale surface structure formation by ion bombardment.

[1] T.C. Kim, C.M. Ghim, H.J. Kim, D.Y. Noh, N.D. Kim, J.W. Chung, J.S. Yang, Y.J. Chang, T.W. Noh, B. Kahng, and J.S. Kim, Phys. Rev. Lett. **92**, 235414 (2006).