Surface deformation of Ga^+ ion collision process via molecular dynamics simulation

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The comprehension of ion beam collision process is very important because ion beam based fabrication process is key technique for nanofabrication. For example, focused ion beam (FIB) milling and ion implantation need the information of surface deformation with atomic scale. However, it is difficult to grasp of atomic scale phenomena caused by ion collision to surface because the moving or removal atomics cannot observe with conventional measurement system. Therefore, molecular dynamics (MD) simulation method is very effective for comprehension of ions and impacted atoms movement. Our previous paper revealed that the hillock height of silicon (Si) surface caused by ion collision and MD simulated height have been coincided. [1] In addition, atomically movement of Si and formation process of surface hillock can be observed via MD simulation. In this paper, transient process of hillock formation to sputtering removal phenomenon can be observed via MD simulation.

Figure 1 shows the MD simulation system and conditions. The substrate was Si (100) plane, ion species was Ga^+, and ion energy was 30 keV. One Ga ion collided with center of Si substrate region. Figure 2 shows the time development of Si surface after Ga^+ collision. In these figures, a groove was formed at the center of collision area, and a lip of a groove was formed a hillock protrusion. And the groove and hillock were increased with time development. In addition, sputtered atoms were observed at after 100,000 steps. Therefore, transient process of collision surface can be grasped via MD simulation. Furthermore, after 400,000 steps snap shot shows sputtered atoms were consisted of not only monomer but also dimer, trimer. Such a result does not recognize at experimental results. Thus, MD simulation is powerful method for comprehension of ion beam collision phenomena. You may think this results show the very large sputtering yield and it is abnormal value compared to experimental value (between 1 and 2 in this system). But, in this MD system, most of Ga ion caused channeling, so probability of collision is very low.

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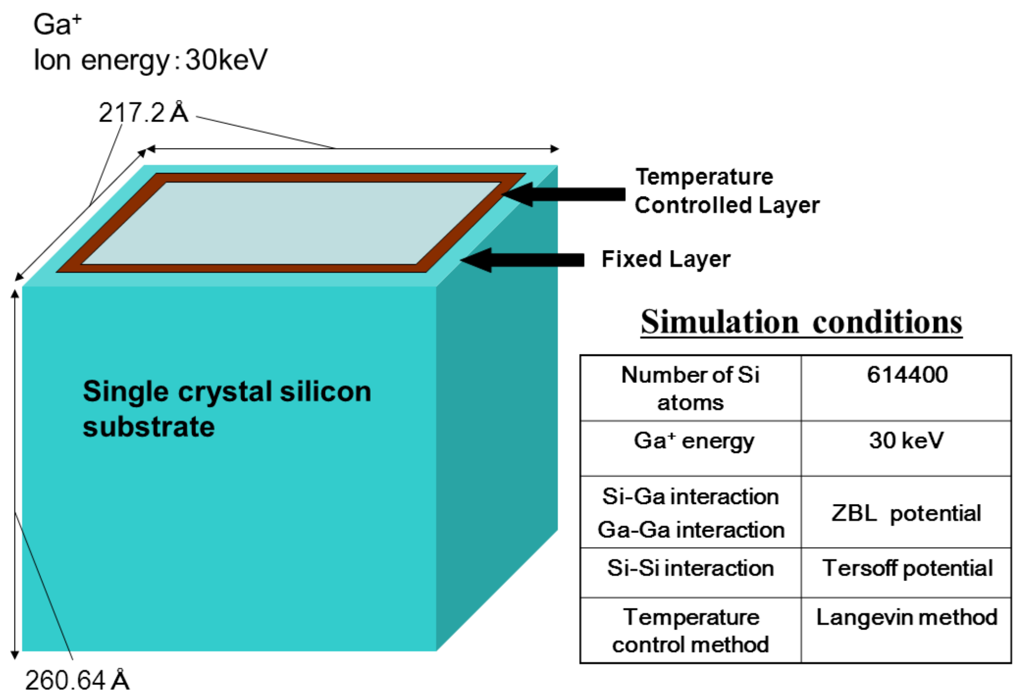
[1]S. Satake, S. Momota, S. Yamashina, M. Shibahara, J. Taniguchi, J. Appl. Phys. **106**, 044910 (2009) 1-4.



Simulation conditions

Number of Si atoms	614400
Ga^+ energy	30 keV
Si-Ga interaction Ga-Ga interaction	ZBL potential
Si-Si interaction	Tersoff potential
Temperature control method	Langevin method

Figure 1: The MD simulation system and conditions.

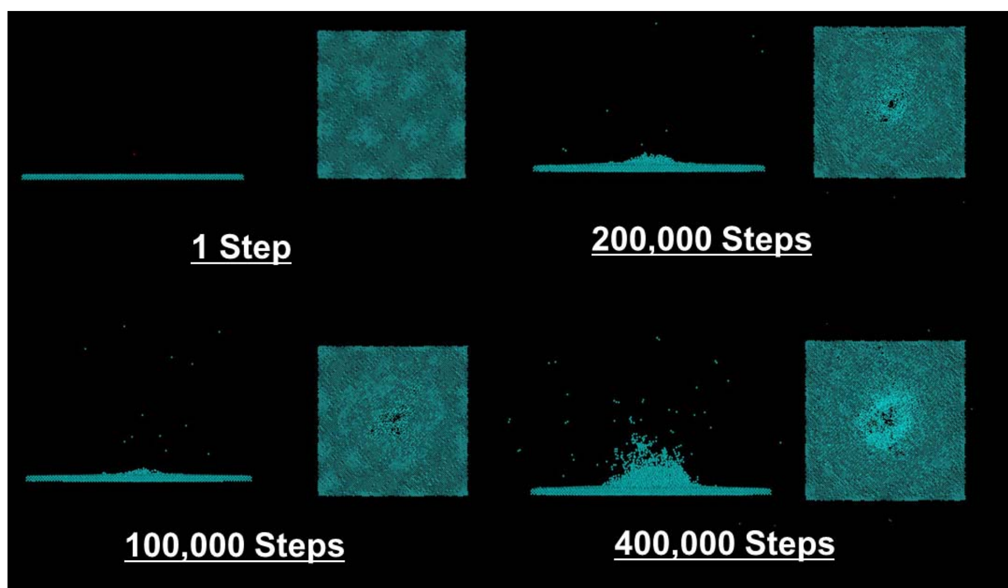


Figure 2: The time development of Si surface after Ga^+ collision.