Study of Ga Ion Induced Amorphization in Si during FIB using TRIDYN simulation

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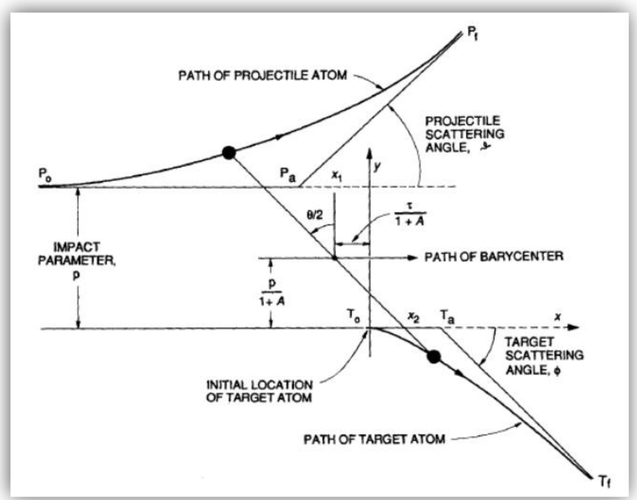
Introduction

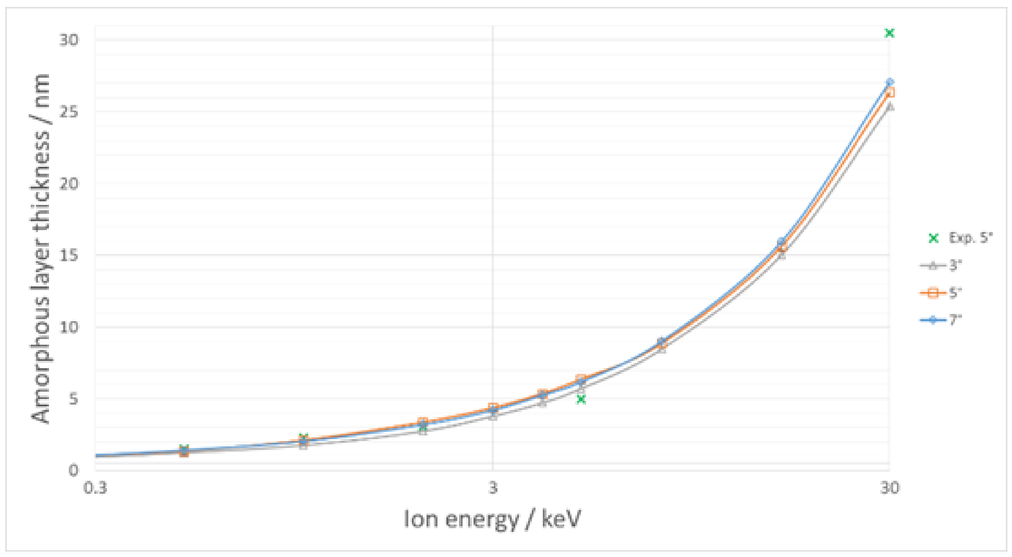
It is well known in the microscopy community that crystalline silicon (c-Si) is partially amorphized during Focused Ion Beam (FIB) preparation. However, the precise mechanism remains not well understood. In this work, as the initial phase of a more sophisticated study, we use a Binary Collision Approximation code, TRIDYN, to simulate the amorphization of c-Si during Ga ion irradiation.

Binary Collision Approximation



In principle, MD simulates the physical movement of atoms and molecules in the context of multi-body effects, whereas in BCA, the ion is approximated to travel through a material by experiencing a sequence of independent binary collisions with sample atoms. A large simulation volume has to be considered for FIB simulation. Therefore a BCA code named TRIDYN is used in this study.

Principles of TRIDYN & Assumptions for Simulation



1. TRIDYN Simulated amorphous Si layer thickness as a function of ion energy for 3˚, 5˚and 7˚ ion impingement angle. Experimental TEM data are also depicted for comparison.

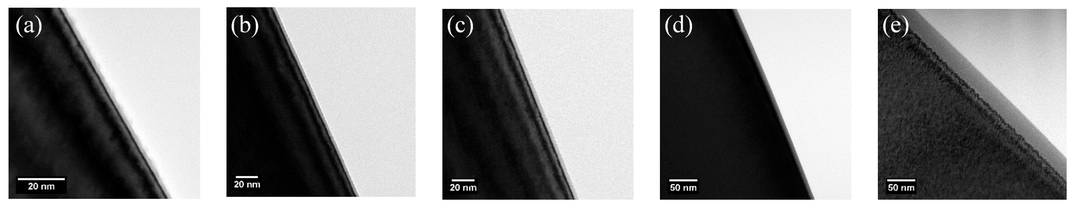
TRIDYN is a computer software that treats the deceleration of ions in solids, and the associated formation of recoil atom cascades in the BCA. It takes into account dynamic alterations of the local composition which arise from the implantation process for ions and the collisional transport movement of target atoms.

(cont.) In this way, phenomena such as implantation profiles, atomic mixing, sputtering and recoil implantation, which occur during high-fluence ion bombardment, can be simulated. Due to the limitation of BCA, TRIDYN is not able to simulate the translation symmetry of crystalline materials. Therefore, alternative criteria for the amorphization of c-Si needs to be established. It has been demonstrated by Monte Carlo simulation and experimental studies that silicon amorphization can be described by host-atom displacement. The threshold displacement for amorphization in silicon is 5Å. On the other hand, it has also been shown that, in terms of atom displacement, MD and BCA do not have a significant difference for <5Å atom displacement. Therefore, it is feasible to use TRIDYN for the simulation of silicon amorphization during FIB, under the mentioned assumptions.

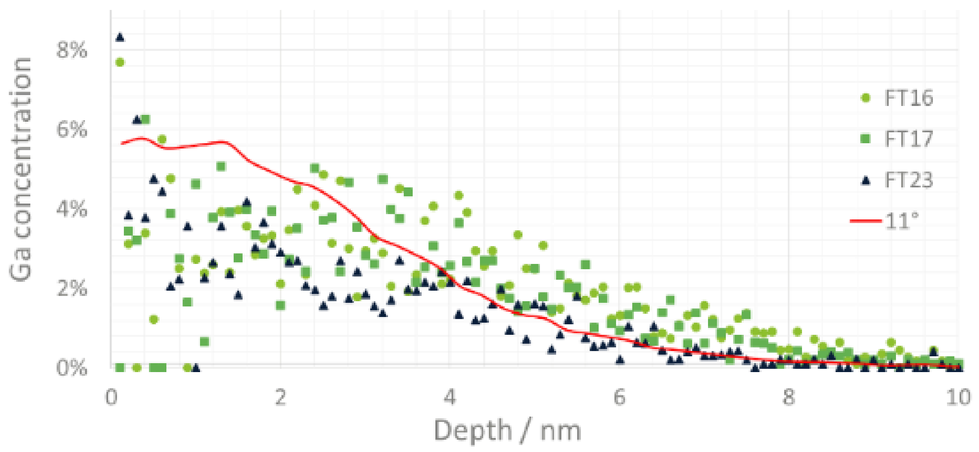
Simulation Results & Comparison to Experiments

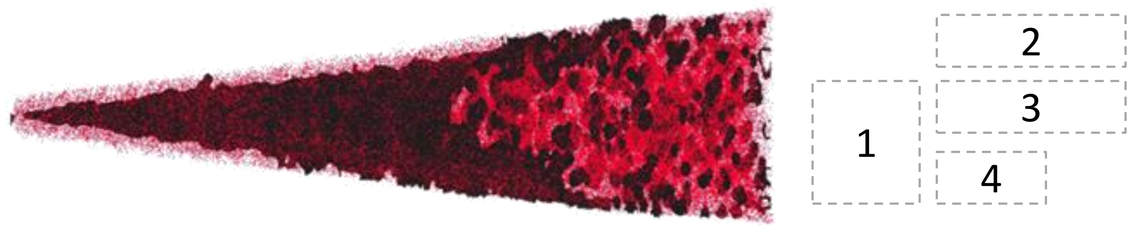
Graph 1 shows the amorphous thicknesses for several simulation parameters. It can be seen that the glancing angle does not have a significant effect here, especially for low energies. In this study, we have employed TRIDYN as a simulation tool to determine the amorphous layer thickness for several FIB conditions, assuming that silicon has an amorphization threshold of 5 Å atom displacement and that BCA is valid for > 5 Å atom displacement.

Preliminary comparison to experimental literature data shows that the simulation data is trustworthy.



2. TEM images of a c-Si cross-section after a 0.5/1/2/5/30kV Ga FIB process show amorphous layer thicknesses of 1.5/2.3/3.1/5.0/30.5nm, from (a) to (e) respectively.





3 & 4. APT determined Ga concentration profiles from three APT samples, with corresponding TRIDYN simulation (3); illustration of APT measurement (Ga: black and Si: red) (4).