Introduction

processes: energy and time scales

atomistic simulation methods

M. Posselt,
Institute of Ion Beam Physics and Materials Research

processes: energy and time scales

ion implantation and subsequent thermal annealing

(i) deposition of the implanted ions and displacement of target atoms during ultrafast ***ballistic processes***

energy: > 100 eV, duration: < 100 fs

(ii) formation of a (meta)stable defect structure after ***fast relaxation***

energy: 1...100 eV, duration: 100 fs ...100 ps

(iii) ***long-term thermally induced processes:***

defect rearrangement, migration, recombination and reduction, interaction between defects and implanted ions

energy: < 1 eV, duration: > 100 ps

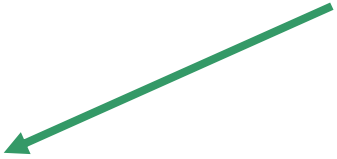
M. Posselt,
Institute of Ion Beam Physics and Materials Research

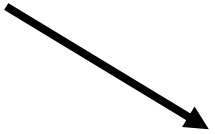
atomistic simulations methods

- based on atomic degrees of freedom
- description of atomic interaction by classical potentials
- semiempirical models for the electronic excitations

processes with different energy and time scales

different types of atomistic simulations





ion implantation

ion-beam induced defect formation

defect migration

M. Posselt,
Institute of Ion Beam Physics and Materials Research

atomistic simulation of ion implantation

ballistic processes energy: > 100 eV, duration: < 100 fs

series of consecutive binary collisions of the moving projectile with the nearest target atom (lattice structure)

repulsive interaction between the projectile and the target atom (screened Coulomb potential)

*semiempirical model for the **electronic energy loss** of fast particles*

*Debye (-Einstein) model for **lattice vibrations***

*phenomenological models for **damage buildup and dynamic annealing***

computer simulations based on the binary collision approximation (BCA), *Crystal-TRIM code*

→range distribution of the implanted ions

→ distribution of atomic displacements

atomistic simulation of ion-beam-induced defect formation

combined simulation method:

ballistic processes
energy: > 100 eV, duration: < 100 fs

BCA simulations

fast relaxation processes
energy: 1...100 eV, duration: 100 fs ...100 ps

Molecular Dynamics (MD)

repulsive *and* attractive interaction between all atoms (classical potential),
semiempirical model for the ***electronic energy loss*** *of fast particles*

→defect types and morphology

M. Posselt,
Institute of Ion Beam Physics
and Materials Research

atomistic simulation of **defect migration**

thermally activated processes

energy: < 1 eV, duration: > 100 ps

Molecular Dynamics (MD)

repulsive and attractive interaction between all atoms (classical potential),

→diffusivity, atomic mechanisms

**M. Posselt,
Institute of Ion Beam Physics
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