

RADIATE Spring School 2021 (28-30 April)

Detailed information on the RADIATE Spring School lectures

Wednesday, 28 April 2021



LECTURE 1

© A. Vantomme

Fundamentals of ion-solid interactions

Lecture by [André Vantomme](#)

KU Leuven, Belgium

Ion beams are widely used in the field of materials science and nano technology, either to modify the material's properties (irradiation), to introduce impurities or dopants (implantation), to remove atoms (sputtering) or to analyze their composition and structure (RBS, channeling, PIXE, NRA...). Hereby, ion energies vary from just a few eV via the keV and MeV region up to several hundreds of MeV. A common feature is that the ion energy is transferred to the material via interaction with the target ions and target electrons. Although based on simple (elastic) atomic collisions, it is often not straightforward to work out the energy transfer from the ion to the solid without making approximations. This lecture will review the basic ion-solid interactions, which result in the concepts of scattering, electronic stopping and nuclear stopping. In turn, these concepts will be the starting point for the modeling, simulations or irradiation studies discussed in the subsequent lectures.



LECTURE 2

© W. Möller

Ion and defect distributions: Monte Carlo simulation

Lecture by [Wolfhard Möller](#)

Institute of Ion Beam Physics and Materials Research, [HZDR](#), Dresden, Germany

The lecture will describe basic principles and applications of Monte-Carlo computer simulations of ion-solid interaction using the binary collision approximation (BCA). An overview of available codes will be given. The model limitations and reliability will be critically discussed. Application results will cover ion implantation, point defect formation, surface sputtering and atomic mixing, as obtained from both static and dynamic simulations, in particular using the [TRIM](#) (one-dimensional static), [TRIDYN](#) (one-dimensional dynamic) and [TRI3DYN](#)¹ (three-dimensional dynamic) codes, the latter in particular with recent results for three-dimensional nanostructures.

¹ W. Moeller, Nucl Instrum Meth B 322, 23-33, [DOI 10.1016/j.nimb.2013.12.027](#) (2014).



LECTURE 3

© F. Djurabekova

Molecular Dynamics simulation of Ion-solid interactions

Lecture by Flyura Djurabekova

University of Helsinki, Finland

In this lecture, I will briefly review the molecular dynamics methods for use in simulations of radiation effects. First we will overview the general algorithms for simulation of equilibrium systems. Then I will explain the physical reasons why these cannot directly be used for simulation of radiation effects, and present the modifications needed for handling high-kinetic energy effects correctly. In the high-energy regime, such as swift heavy ions, we overview the existing

models of extending the classical molecular dynamic methods to include effects of electronic excitations. At the end, we will also discuss the complications associated with modelling complex radiation effects and challenges, which remain to be resolved.

Thursday, 29 April 2021



LECTURE 4

© K. Lorenz

Tailoring material properties by ion implantation

Lecture by Katharina Lorenz

Instituto Superior Técnico, Lisboa, Portugal

Ion beams can be used to tailor materials properties, for example, by the synthesis of new phases, doping, intermixing, nanopatterning or defect engineering. After a short introduction to the wide field of applications of ion beam modification of materials, this lecture will focus on ion implantation in semiconductors. With this technique, electrical, optical or magnetic dopants can be easily incorporated into a semiconductor crystal. But where exactly in the lattice are the implanted ions incorporated? And how does implantation damage – inevitably formed during the bombardment with energetic ions – impair materials and device properties? Interestingly, some answers can be provided by ion-solid interactions themselves. In particular, we will discuss the measurement of defect profiles and of the lattice site of the implanted ions by Rutherford Backscattering Spectrometry/ion channelling.



LECTURE 5

© E. Wendler

Empirical modelling of ion-beam induced damage formation

Lecture by Elke Wendler

Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Germany

This lecture gives an overview of empirical models for describing ion-irradiation-induced defect production and accumulation, and amorphisation. Model calculations illustrate the effect of parameters occurring in the models presented. Various models that represent similar processes are compared with each other. The use of such empirical models may help in understanding of the physical processes during ion irradiation of materials. Further, when a sufficient number of data is available, the obtained model parameters can be analysed on the base of the primary energy deposited by the implanted ions to the atoms of the respective material. This could be used for predicting the damage to be expected for chosen implantation conditions. However, we will also advise you of misinterpretation in the value of such model calculations, because the formulae are built according to possible mechanisms which we guess from our experimental data.



LECTURE 6

© J. Olivares

Optical waveguide engineering by ion beams

Lecture by José Olivares^{1,2}

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Optical waveguides are key elements of many photonic devices, which in turn are essential for the advance of the information society. In addition they can be combined with other singular useful structures like for example nanoparticles with plasmonic properties. Ion irradiation provides a general and flexible method to fabricate or further tune optical waveguides, showing several advantages over the alternative techniques. Initially, optical devices are manufactured using low-energy light ions (H and He at a few MeV), taking advantage of the effects caused by nuclear damage. Later on, the use of the electronic excitation provided by high energy heavy ions (or swift heavy ions for $E > 1$ MeV/amu) has been developed, allowing to produce novel micro- and nanostructures that make possible to achieve higher optical confinement as needed for example for optical microrings, or nanopore structures.

Friday, 30 April 2021



LECTURE 7

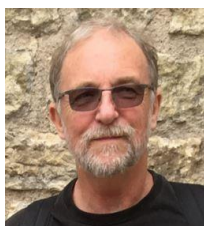
© M. Sequeira

Swift Heavy Ion irradiation of materials

Lecture by Miguel C. Sequeira

Instituto Superior Técnico, Lisboa, Portugal

In this lecture, we will address the interaction of Swift Heavy Ions with materials. We will start by looking at the characteristics of this class of strongly ionising radiation. Its differences from other types of radiation, its origins, its effects and its technological importance will be discussed. Afterwards, we will examine the interaction dynamics leading to the observed effects, first from a thermodynamics perspective and latter using atomistic simulations. Special focus will be given to the interaction with semiconductors, namely with group-III nitrides, due to their widespread applications.



LECTURE 8

© S. Donnelly

Real-Time Studies of Ion-Solid Interactions

Lecture by Steve Donnelly

School of Computing and Engineering University of Huddersfield, Huddersfield, UK

In-situ ion irradiation within a Transmission Electron Microscope (TEM) has been used since the 1960s in a number of dedicated facilities around the world, to study ion-solid interactions. This lecture will provide examples of research in which the ability to observe, at high magnification, the changes taking place in specimens under ion irradiation, in real time and at a range of temperatures, can provide powerful insights into mechanisms responsible for the defect structures, phase changes and other morphological changes that occur under ion irradiation. Examples will be given of experiments in which the effects of individual ion impacts can be observed. The lecture will also discuss the use of in-situ ion irradiation to simulate neutron-induced damage in a variety of materials in the context of materials for both fission and fusion reactors.



LECTURE 9

© R. Webb

Towards Single Ion Implantation

Roger Webb is the Director of the UK National Ion Beam Centre (a collaboration between the Universities of Huddersfield, Manchester and Surrey) and has led the Surrey University Ion Beam Centre (SIBC) since 2004. The SIBC has a broad portfolio of users, coming from three principal funding streams. About one third of the IBC support comes from UK research councils, one third from the EU and one third from industry, providing a relatively robust funding model. He is a founding member and chair of the international committee of the Computer Simulation of Radiation Effects in Solids

(COSIRES) and Radiation Effects in Matter (REM) conference series and he is the UK representative on the European Conference on Accelerators and Applied Research Technology (ECAART) and the International Ion Beam Analysis (IBA) conference series. He has been a member on a number of IAEA advisory panels relating to ion beam interactions with materials as well as secretary to the UK Institute of Physics Ion and Plasma Surface Interactions group. He was co-developer of the Ion Beam Analysis package (used world-wide) WiNDF. He has published over 230 refereed papers and book chapters (h-index 34, >4500 citations) and made more than 200 presentations at conferences and workshops worldwide. He leads research programmes advancing new methods for ion beam analysis (e.g. pioneering a sub-micron ambient mass spectrometry technique, MeV-SIMS, leading an IAEA coordinated research programme as well as an EU MC-ITN Work Package in this area) and ion implantation (e.g. the development of purpose built single ion implanters for deterministic implantation and quantum technology applications – SIMPLE). He has >40 years of experience in the application and understanding of ion-solid interaction given to the interaction with semiconductors, namely with group-III nitrides, due to their widespread applications.