UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Theory and Modeling of Epitaxy

2425-116R-M01

Title

Theory and modelling of epitaxy

Teacher(s)

Prof. Roberto Bergamaschini
Prof. Francesco Montalenti

Language

English

Short description

Epitaxy, i.e. the ordered growth of one material on top of a crystalline substrate, is a key process in materials science, ubiquitously used for the fabrication of high-quality films and hetero-structures of complex design. This course provides a general introduction to the physics of epitaxial growth, offering an overview of the key thermodynamic and kinetic factors driving the formation of thin-films rather than three-dimensional micro- or nano-structures during. While the focus of the course will be mostly on the theoretical aspects behind the growth, the content will be discussed by an applied perspective, constantly related to the experimental observations. The purpose is then two-fold: 1) to provide a comprehensive overview of current understanding and methods as a

starting point for further, more specific, investigations of the growth dynamics; 2) to provide useful guide-lines for the interpretation and tuning of experiments.

The course is divided in two modules.
A) GENERAL INTRODUCTION TO EPITAXY AND CONTINUUM METHODS (prof. Roberto Bergamaschini)
In this module, epitaxial growth is inspected from a macro/mesoscopic point-of-view. After a review of the basic concepts of epitaxy, including experimental methods and applications, the key thermodynamic aspects describing the crystal morphology and stability for both homoepitaxial and heteroepitaxial systems will be discussed, including elastic and plastic relaxation effects.

B) ATOMIC-SCALE MODELLING AND MACHINE LEARNING APPROACHES (prof. Francesco Montalenti)
This module focuses on the modelling of epitaxy at the atomistic scale, analysing the elementary mechanisms leading to the growth and highlighting the role of stepped surfaces in the evolution dynamics. The classical modelling techniques of Molecular Dynamics and Kinetic Monte-Carlo will be discussed for this purpose. Finally, novel approaches exploting Machine Learning techniques will be presented.

CFU / Hours

2 CFU / 16 hours

Teaching period

From June 23rd to July 4th, 2025

Sustainable Development Goals

QUALITY EDUCATION