

# UNIVERSITÀ DEGLI STUDI DI MILANO-BICOCCA

# SYLLABUS DEL CORSO

# **Theory and Modeling of Epitaxy**

2425-116R-M01

#### **Titolo**

Theory and modelling of epitaxy

### Docente(i)

Prof. Roberto Bergamaschini Prof. Francesco Montalenti

## Lingua

**English** 

#### **Breve descrizione**

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 parts. In the first, 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.

The second part focuses on 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 to parametrize the interaction potentials will be introduced.

#### CFU / Ore

2 CFU / 16 hours

### Periodo di erogazione

Dal 23 Giugno al 4 Luglio 2024

#### **Sustainable Development Goals**

ISTRUZIONE DI QUALITÁ