

ABSTRACT

Diploma work: 83 pages, 17 figures, 23 literature sources.

Purpose of research: the development of advanced mathematical and computer techniques and skills for the use of software tools for calculation of thin film deposition process.

Object of research: SiC, SiO₂ crystal substrates and a thin layers of SiC, SiO₂ .

Experimental methods: computer experiment - modeling methods DFT thin film deposition process (PVD, CVD).

Practical value: Modeling processes of growth thin films can help to deeply learn the basic microscopic mechanisms, and the impact of process parameters such as pressure, temperature, etc. in the resulting atomic structure and kinetics of processes that occur during the deposition of a thin layer on a substrate to optimize the manufacturing processes of thin-film structures.

THIN FILM; COMPUTER MODELLING; VAPOR DEPOSITION; MOLECULAR
DYNAMICS; VISUALIZATION; SUBSTRATE; FREQUENCY OF
DEPOSITION; CRYSTALL SiC; RESERVOUR; DEPOSITION ATOM; ACTIVE
SURFACE.