KN0200

Pathways for the preparation of technologically important metal oxides

Jiri Houska

University of West Bohemia, Plzen, Czech Republic

jhouska@kfy.zcu.cz

The growth of metal oxide thin films is studied by molecular dynamics (MD) simulations. The overall aim is to define pathways for the low-temperature preparation of desired crystalline phases. Because the success and reliability of classical MD in general and growth simulations in particular strongly depends on the interaction potential (force field), the first part of the contribution presents an algorithm for the development of interaction potentials optimized for the growth simulations. Most importantly, and contrary to most of the literature, the newly developed potentials correctly reproduce the preferred coordination number of individual elements. The second part of the contribution uses the reliable interaction potentials in order to investigate the relationships between the (i) process parameters such as energy delivered into the growing films (E), energy distribution function of the particle flux (EDF), temperature (T) and growth template and (ii) film characteristics such as densification, crystal nucleation, uninterrupted crystal growth and its dependence on the crystal orientation. The results show that and how the characteristics of individual phases depend not only on E (i) per fast atom (ion) or (ii) per any atom, but especially on the (iii) EDF (particularly the fraction of fast atoms in the particle flux) and (iv) mass (momentum) of fast atoms. There is a difference between conditions for crystal nucleation (often difficult, T□dependent) and for uninterrupted growth of existing crystals (for some phases and orientations much easier and almost T□independent). Optimum EDFs which allow uninterrupted growth of densified difficult-to-prepare phases at as low T and/or E as possible are characterized by (i) narrow EDF around a material-dependent optimum value and (ii) high momentum delivered into the growing films.

Keywords
molecular dynamics
crystal nucleation
crystal growth
metal oxides