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Molecular dynamics simulations and experimental study of complex oxide thin film growth

Violeta Georgieva[1], Marta Saraiva[2], Neerushana Jehanathan[3], Gustaaf Van Tendeloo[3], Diederik Depla[2], Annemie Bogaerts[1]

[1]University of Antwerp, Wilrijk-Antwerp, Belgium [2]Ghent University, Ghent, Belgium [3] University of Antwerp, Antwerp, Belgium

violeta.georgieva@ua.ac.be

The crystallinity of simulated $Mg_xM_yO_z$ (M=Al, Cr, and Y) thin films by a molecular dynamics (MD) model is studied with a variation in the stoichiometry of the thin films at operating conditions similar to the experimental conditions of a dual magnetron sputter-deposition system. The Mg metal content in the film ranges from 100% (i.e. MgO film) to 0%, (i.e. M_2O_3 film) [1, 2]. A classical ionic potential with formal charges describes the interactions between atoms. The radial and angular distribution functions of the films and the coordination numbers of the cations are calculated in order to analyze the film structure. The results are compared with X-ray diffraction (XRD) and transmission electron microscopy (TEM) analyses of experimentally deposited thin films by the dual magnetron reactive sputtering process.
Both simulation and experimental results showed that the structure of the Mg-M-O film was varying from crystalline to amorphous when the Mg concentration decreases. The crystalline Mg-M-O films have a MgO structure (cubic, S.G. Fm3m) with M in solid solution. The transition from a crystalline to an amorphous film is observed at 50, 40 or 70% Mg metal ratio when M is Al, Cr or Y, respectively.
Another observation, which is related to the cation radius, was the change of the lattice parameter of MgO due to the presence of the doping element. It was observed that replacing Mg^{2+} by a cation with a smaller radius such as Al^{3+} or Cr^{3+} resulted in a decrease in the lattice parameter [2]. The opposite trend was noticed when a larger cation such as Y^{3+} replaced the Mg^{2+} cation.
Influence of the substrate temperature on the Mg-Al-O film structure has also been investigated. It was found that the transition point to amorphous structure shifted to lower Mg concentration when increasing the substrate temperature, which was also confirmed by the experiment.
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Keywords
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