E-MRS 2009 spring meeting

Strasbourg, 8.-12.6.2009

Molecular dynamics simulations of the sputtering of SiC and Si_3N_4

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Thin films of silicon carbide (SiC) and silicon nitride (Si_3N_4) have been deposited on Si (100) substrates by r.f. magnetron sputtering in Ar atmosphere. In parallel molecular dynamics simulations of the sputtering of β-SiC and β-Si_3N_4 by Ar atoms were performed using IMD and Materials Explorer software with a combination of the Tersoff and the Ziegler-Biersack-Littmark (ZBL) potential in order to get more insight into the sputter process, the film deposition, the growth and the phase formation. In the experiments the substrate temperature and the bias voltage (0 to -40 V) have been varied to investigate the possibility for the deposition of nanocrystalline films and to study the influence of these deposition parameters on composition, constitution and mechanical properties of these films. The films have been characterized by EPMA, XRD, FTIR and AFM. Hardness and residual stress have been investigated by nanoindentation and wafer bending. In the MD simulations the sputter yield was determined for both materials as a function of the energy of the incident Ar atoms (in the interesting range for PVD deposition, i.e. 20-1000 eV). The results of the MD simulations have been compared with our own experiments and data from the literature and a good agreement has been found. Furthermore, the trajectories of the Ar atoms, the damage caused by collision cascades inside the crystal and the ranges of Ar ions and the different ratios of the sputtered species were investigated.