Molecular dynamics simulations of the sputter deposition process of silicon carbide on silicon and comparison with experiments

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Thin films of silicon carbide (SiC) have been deposited on silicon substrate by rf magnetron sputtering from a SiC target in pure Ar atmosphere. In parallel the sputter deposition process has been simulated by the method of molecular dynamics, using the ITAP Molecular Dynamics program package. Both Si-Si and Si-C interactions within the bulk and at surface positions are well described using the Tersoff potential. Considering the fact that the Tersoff potential overestimates the melting point of silicon as well as of silicon carbide, the coating process was simulated at substrate temperatures of 1000 K and 3000 K.

In the experiments the substrate temperature has been varied between 900 °C and 100 °C to find the minimum temperature that is needed to deposit nanocrystalline β-SiC films under the applied sputter conditions (ceramic SiC target, 300 W rf power, 18 cm target-substrate distance, 0.26 Pa total gas pressure). The grown films have been characterized by electron probe micro-analysis, x-ray diffraction, atomic force microscopy, and both Raman and FTIR spectroscopy. Hardness and residual stress have been investigated by nanoindentation and wafer bending.

The sputter deposition process was simulated by a method, where silicon and carbon atoms are created over the specimen and are being shot towards the specimen with specified kinetic energies. For the kinetic energies, 1.5 eV, 3 eV and 6 eV were used, corresponding to one quarter, one half and full surface binding energy of silicon carbide. Moreover three different Si crystal surfaces were used for the deposition of silicon carbide: Si(100), Si(110) and Si(111). An additional parameter, controlling the interaction between the add atoms and the substrate. Simulating an infinite silicon bulk and a thin film of silicon carbide, the choice of constant temperature or an NVT ensemble is a good choice, using silicon bulk as the heat bath. In order to maintain their kinetic energies, the add atoms were integrated with using NVE ensemble. The switching from the NVE to an NVT ensemble for the add atoms as they reach the substrate is controlled by out additional parameter introduced above. The value equal to the one half of the mean potential energy of the silicon bulk, corresponding to two free bonds of the surface atoms, was used for this parameter. At last simulations for two different coating rates, 1 atom/ps, and 0.1 atom/ps were performed. In general, the crystallinity was lower at higher coating rates.

After the simulations analysis of the coating properties and structure was performed by e.g. common neighbour and coordination number analysis, put into relation with each coating parameter and compared with the experimental data.