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Molecular dynamics simulations of the sputtering process of silicon and the homoepitaxial growth of a Si coating on silicon

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The main research goal of this work is production and optimization of thin silicon films on a silicon substrate. Experimentally, thin silicon films can be deposited by dc magnetron sputtering of a silicon target in Ar atmosphere. Variations of Ar-ion rate and impact energy result in different sputter yields and are important for the formation of silicon coatings. All variables such as vacancy, migration and surface binding energy were analysed by the method of molecular dynamics simulations, using the ITAP Molecular Dynamics (IMD) programme package. A Tersoff potential was used to simulate Si-Si-interactions within the bulk and on the surface while the interaction with Argon was described by the Ziegler-Biersack-Littmark (ZBL) potential. At first, the vacancy energy of silicon was analysed by comparing two equivalent specimens with and without vacancy inside. Secondly, the migration energy was defined as the energy barrier between two neighbouring lattice sites, one occupied, other vacant. The knowledge of these energy values is important for the understanding of the penetration depths of argon ions and the front sputtering of silicon. For the process of back sputtering of silicon, the surface binding energy with and without the recombination of the crystal surface was analysed. Using these energy values, the sputter yield of silicon was determined as a function of ion impact energy (20-1000 eV) and impact site on the Si (100), (110) and (111) surfaces by IMD and commercial Materials Explorer 4.0 (ME) software from Fujitsu Ltd.. These simulation results have been compared with experimental values as determined by Ar ion etching in a microwave plasma and measurement of the etch depth. A good agreement between experiments and simulations has been found as shown exemplarily in Fig. 1. for the Si (100) surface.

The coating process was simulated by a method, where one atom after another is being shot towards the specimen with specified kinetic energy. Different types and vales of input parameters were used, such as silicon impact energy (1.5-

6 eV), rate (1 atom/fs, 0.1 atom/fs), substrate temperature (1000 K, 3000 K), and crystal surfaces (100), (110), (111).

The quality of the produced coatings and its dependence on each of the parameters stated above was analysed. Under specific parameter settings homoepitaxial growth of silicon coatings on silicon was possible, as shown in Fig. 2.

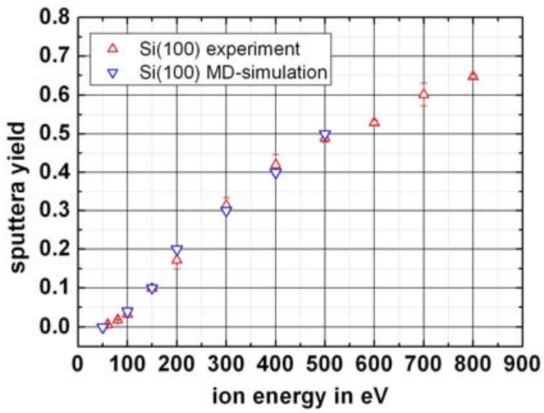

Fig.1 Silicon sputter yield as a function of argon impact energy: comparison between experiment and molecular dynamics simulation

Fig.2 Silicon substrate (left), amorphous silicon coating at high deposition rate (middle), crystalline coating at low deposition rate (10% of the deposition rate in the middle example)

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