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Sputtering of MoS2 by argon atoms

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A new binary Monte Carlo (MC) model of sputtering based on quantum mechanical cross sections is presented. Instead of traditional MC programs based on classical calculation of a scattering angle our model uses quantum-mechanical differential atom-atom elastic cross section. This helped to improve description of small - angular scattering of an incident atom on a recoil one. The developed model works on 3D maps of solid and allows to obtain both 3D images of films at every time step of sputtering process and sliced distribution of trapped atoms and matrix components in any 3D direction.
The model was used to model sputtering of ultra-thin MoS_2 films under Ar bombardment. Dependencies of Mo-S, Mo-Ar, S-Ar atomic interaction potentials on distances were obtained with density functional theory (DFT) calculations and compared to empirical Stillinger-Weber Mo-S potential, which was successfully applied for molecular dynamics (MD) modeling of MoS_2 monolayer properties, and to semi-empirical Moliere and ZBL potentials that are usually used for describing the interaction between incident Ar ions and atoms in solid medium in MC and MD simulations. Some parameters of the presented MC model, e.g. surface binding energy, were estimated with the DFT method. The obtained results are in reasonable agreement with literature data. The authors expect the developed code will be of help in plasma processing industry.

Keywords
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