A remaining challenge in making fusion energy commercially available is the development of suitable construction materials for the reactors. These materials have to withstand the extreme conditions found in a fusion reactor, e.g. high temperatures and radiation, that can drastically change the material’s properties. One important task in developing improved fusion reactor materials is studying the interaction between the plasma and the plasma-facing material in the reactor.

The fuel of future fusion reactors will be hydrogen isotopes confined by magnetic fields in a plasma. However, due to the imperfect plasma confinement impurities originating from the wall material will contaminate the plasma (in addition to the fusion reaction product helium). The erosion of wall materials leads among others to the formation of mixed materials, e.g. to the formation of tungsten-carbide in the divertor region of the experiment fusion reactor ITER due to the presence of tungsten and carbon fibre composite plates.

Results of molecular dynamics simulations of cumulative deuterium co-bombardment with C, W, He, Ne, or Ar impurities on crystalline tungsten-carbide are presented. The simulations were performed using a reactive bond-order potential for the W-C-H system, that can both describe pure materials and compounds reasonably compared to experimental and ab initio data [1]. The studied bombardment energy range was 100 to 300 eV, i.e. in the region with the highest carbon sputtering yields in the low energy regime [2]. Effects of the impurities on the sputtering yields and preferred sputtered molecules are discussed. During the the bombardment process accumulation of deuterium and noble gases in the sample was observed, resulting in amorphization and blistering.