Molecular dynamics study of hydrogen isotopes migration in amorphous silica

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Fused silica is a material of interest due to its increasing number of applications in many different technology fields. In thermonuclear fusion it is a key component in a number of diagnostics of the Safety and Control Systems of the ITER machine as well as in the final focusing optics of lasers for NIF.

Materials properties of interest (optical absorption, radioluminescence, mechanical properties, etc) are closely related to the presence of defects. These defects can be generated directly by irradiation or by the presence of impurities in the material. Hydrogen is an ubiquitous impurity in this material and, moreover in a fusion reactor environment this material will be exposed to energetic hydrogen isotopes. Hydrogen isotopes will be deposited also on the surface of the fused silica components coming from the reaction chamber. On the other hand, some experimental results show that radiation damage can be different depending on hydrogen content, indicating that a detailed knowledge of the hydrogen role in fused silica should be fully understood.

In this work we present molecular dynamics simulations to study the effects of different hydrogen isotopes in this material and their interaction with defects. The interatomic potential developed by Feuston and Garofallini has been used in these studies. The diffusion coefficients and mechanisms of H mobility in fused silica has been calculated and compared with those existing in the literature.

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