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Multiscale Modeling of Materials: Light Species Dynamics in nano-W and EOS of Hydrogen

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Multiscale Modeling (MM) demonstrates its important role in the deep understanding of physics mechanisms involved in materials behavior under extreme conditions. Damage of materials by neutrons and ion irradiation in Fusion Systems is progressively better characterized by using a combination of experiments and simulation. It is also possible to give the conditions of Hydrogen (EOS) when cryogenic and under high pressures, such as happens in first states of fuel in Inertial Fusion targets.
Benefits from MM are presented related to the diffusion of light species (H, He) in W and nanocolumnar W and EOS of H and H-Be.
A comparison between Binary Collision Approximation (BCA) and Molecular Dynamics (MD) has been performed to conclude its influence in the defects formation and their diffusion in W depending on the type of irradiation. Ion and neutron irradiation show a very different behavior. The H retention because of grain boundaries size and concentration has been modeled both with Density Functional Theory (DFT) and Object Kinetic MonteCarlo (OKMC) (fed with parameterization from DFT), and compared with experiments in nano-W and coarse-grained W (CGW). Grain Boundaries acts as preferential paths for H diffusion; a combination of H and vacancies (more concentrated in nano-W than CGW) in HV are on the core of the explanation. When studying dependence of the hydrogen diffusion coefficient on grain size and hydrogen concentration by MD calculations, it is coherently demonstrated a smaller value for nano-W than CGW. Using OKMC (parameterization from DFT), we study the influence of a high grain boundary density on the amount, size and distribution of defects produced by pulsed helium irradiation in tungsten, in both monocrystalline and nanocrystalline tungsten. In nano-W the total elastic strain energy remains almost constant with the increasing number of pulses, contrary to its increase in monocrystalline tungsten.
Related to H and H-Be impurities under extreme conditions, "ab initio", Quantum Molecular Dynamic and Mechanical Properties calculations are performed to study the relation between the structural phase transitions and sound velocity in solid molecular hydrogen at 15K pressures from 0,01 to 160 GPa. The structural difference of solid molecular hydrogen pure and solid molecular hydrogen with beryllium is remarked with differences in elastic constants.

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