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Development of a potential model for tritium behavior in tungsten

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Tritium accumulation in plasma facing components such as tungsten is considered as an important fusion engineering issue, because (1) it affects the feasibility and economy of tritium fuel cycle and (2) the accumulation amount is vital information to make a plasma operation scenario that meets a radiation-safety regulation limit of tritium. Therefore, experimental data on the tritium accumulation has been largely acquired in the last decade. In order to predict the tritium accumulation in a fusion environment using those experimental data, it is needed to fill gaps between fusion reactor conditions and experimental conditions in tritium flux, neutron flux and fluence, etc, based on detailed understanding of the tritium behavior in damaged tungsten. Computational simulations in an atomic scale are expected to contribute to revealing the tritium behavior.

Among several available computational methodologies, classical molecular dynamics (MD) method has an advantage in an atomic scale resolution with a relatively low computational cost. MD can deal with millions of atoms, and thus can simulate complex defects, such as ones composed by multiple vacancies and multiple tritium atoms. The low computational cost is realized by describing interatomic interactions with simplified model functions, so-called potential model. Due to this simplification, however, the accuracy of simulation results depends on the quality of potential model. For tungsten-tritium systems, two potential models [1, 2] have been widely utilized in MD simulations. However, their descriptions of tritium-vacancy interaction are not necessarily satisfactory, which motivates us to develop a new potential model.

Thus, our group try to develop a new tungsten-hydrogen potential model which can adequately reproduce a great number of ab-initio calculation results on energy and force in IAEA-CRP activity. The model function is composed by multiple basis functions [3] and their coefficients are uniquely determined by solving linear simultaneous equations. In this presentation, first, formulas to represent two-body inteaction model and embedd-atom model (EAM) will be introduced. The validity and limitation of the methodology will be discussed with results of validation test on magnesium oxide, where error convergences to the number of reference ab-initio calulation data and to the number of involved basis functions are analyzed and then the effect of EAM term on reduction of the errors will be shown. Then, our plan on which tungsten-hydrogen systems are considered in reference ab-initio calculations will be explained. Finally, the quality of a potential models which were preliminary constructed for tungsten and tungsten-hydrogen systems with available ab-initio data will be is presented

References: [1] N. Juslin et al., J. Appl. Phys. **98**, 123520 (2005); [2]X.C. Li et al., J. Nucl. Mater. **408**, 12 (2011); [3] C. M. Handley and J. Behler, Eur. Phys. J. B **87**, 152 (2014).