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# Development of Fe-Ni-Cr-H Interatomic Potential

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**Abstract:** Experiments indicated that tritium permeation in 316 austenitic stainless steel is enhanced by a factor of ~2-5 after irradiation as compared to ex-reactor results. Molecular dynamics simulations need to be performed to understand this enhancement. Such molecular dynamics simulations cannot be performed due to the lack of an Fe-N-Cr-H(T) interatomic potential. Here based on density functional theory calculations, we have developed an Fe-Ni-Cr-H embedded atom method potential. We demonstrate that for the Fe-Ni-Cr part, our potential enables stable molecular dynamics simulations of both austenitic and ferritic stainless-steel alloys at high temperatures, accurately reproduces the experimental stacking fault energy of these alloys over a range of compositions, gives reasonable elastic constants, energies, and volumes for various compositions. For the H-metal interaction part, our potential captures accurately diffusion energy barriers, swelling volumes, and relative energies as a function of background metal composition. Furthermore, our potential prescribes negative H-H interactions in stainless steels as observed from density functional theory calculations. Stringent molecular dynamics simulation tests have been performed to successfully derive H diffusion energy barriers from Arrhenius plots. These results suggest that our potential provides a robust atomistic approach to study H(T) permeation in stainless-steels that can account for all local statistical effects such as variations of metal species and irradiated defects near the atomic jump paths.

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