Nano simulation study of elastic constant in Fe-Ni-Cr alloy doped C

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ABSTRACT

We proposed the microstructure-based multiscale simulation of duplex stainless steel by using phase-field (MICRESS) and finite element simulation (ABAQUS) software. In the simulations, it is key to use accurate elastic constant of the steel. However, because the elastic constant depends on chemical composition of the steel, it is difficult to obtain the elastic constant for multicomponent steels from database and datebook. In this study, we calculated the elastic constant of the duplex stainless steel (Fe-Ni-Cr-C alloy) using first principle calculation and molecular dynamics simulation software: VASP and LAMMPS. The first principle calculation was used to verify the EAM potential function used for the molecular dynamics simulation in order to lead to the same result each other in the simple crystal structure of alloy. Large-scale atomic structure model was used in order to obtain the elastic constant in the condition of dilute carbon composition in the steel. The calculated elastic constant was good agreement with experimental one.

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