Stability of a single He in interstitial sites of $Fe_{(1-x)}$-Cr_x alloys: A first-principles study

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The Low-activated ferritic/martensitic steels are proposed as structural material in fusion reactors due to its greatest maturity in technology. In fusion environment, huge amounts of He atoms are produced by transmutation along with structural damage in the structural materials. The production of insoluble He is a special issue for the fusion environment and therefore an important problem in the design of fusion reactor. Using density-functional theory in combination with the exact muffin-tin orbital (EMTO) as well as vienna ab-initio simulation package (VASP), we have calculated the total energies of a single He in BCC Fe supercell of 16 atoms ($2 \times 2 \times 2$) as function of volume of supercell. The two methods give the same energy trend with increasing the volume of spuercell and also give the same energy difference between two different volumes. Based on this result, we further investigated the alloy effect on the stability of single He atom in interstitial sites by EMTO. Our results show the formation energies of a single He in interstitial sites increase with increasing Cr content in $Fe_{(1-x)}$-Cr_x alloys (x=0, 0.09, 0.15, 0.5, 0.95, 1).

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