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Understanding the mechanical properties of reduced activation steels

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Abstract

Reduced activation ferritic/martensitic (RAFM) steels are structural materials with potential application in Generation-IV fission and fusion reactors. We use density-functional theory to scrutinize the micro-mechanical properties of the main alloy phases of three RAFM steels based on the body-centered cubic Fe-CrWVMn solid solution. We assess the lattice parameters and elastic properties of ferromagnetic α-Fe and $Fe_{91}Cr_9$, which are the main building blocks of the RAFM steels, and present a detailed analysis of the calculated alloying effects of V, Cr, Mn, and W on the mechanical properties of $Fe_{91}Cr_9$. The composition dependence of the elastic parameters is decomposed into electronic and volumetric contributions and studied for alloying levels that cover the typical intervals in RAFM steels. A linear superposition of the individual solute effects on the properties of $Fe_{91}Cr_9$ is shown to provide an excellent approximation for the *ab initio* values obtained for the RAFM steels. The intrinsic ductility is evaluated through Rice's phenomenological theory using the surface and unstable

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