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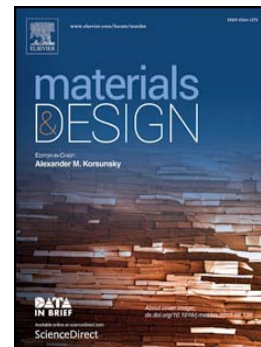
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Xiaojie Li, Xiaoqing Li, Stephan Schönecker, Ruihuan Li, Jijun Zhao,  
Levente Vitos

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# Understanding the mechanical properties of reduced activation steels

Xiaojie Li<sup>a,b</sup>, Xiaoqing Li<sup>b,\*</sup>, Stephan Schönecker<sup>b,\*</sup>, Ruihuan Li<sup>c</sup>, Jijun Zhao<sup>a,\*</sup>, Levente Vitos<sup>b,d,e</sup>

<sup>a</sup>Key Laboratory of Materials Modification by Laser, Electron, and Ion Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

<sup>b</sup>Applied Materials Physics, Department of Materials Science and Engineering, KTH - Royal Institute of Technology, Stockholm SE-10044, Sweden

<sup>c</sup>Institute of Mold Technology, Changzhou Vocational Institute of Mechatronic Technology, Changzhou 213164, China

<sup>d</sup>Department of Physics and Astronomy, Division of Materials Theory, Box 516, SE-75120 Uppsala, Sweden

<sup>e</sup>Research Institute for Solid State Physics and Optics, P.O. Box 49, H-1525 Budapest, Hungary

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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  $\alpha$ -Fe and Fe<sub>91</sub>Cr<sub>9</sub>, 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<sub>91</sub>Cr<sub>9</sub>. 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<sub>91</sub>Cr<sub>9</sub> 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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\*Corresponding author

Email addresses: xiaoqli@kth.se (Xiaoqing Li), stesch@kth.se (Stephan Schönecker), zhaojj@dlut.edu.cn (Jijun Zhao)

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