

Abstract Submitted
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***Ab-initio* calculations on the energetics of vacancies in α -Fe under strain field**¹ ERIC SANCHEZ, SERGIO OROZCO, ZHENGZHENG CHEN, NICHOLAS KIOUSSIS, Department of Physics and Astronomy, California State University Northridge — *Ab-initio* calculations have been carried out to investigate the energetics of vacancies in α -Fe under external deformation. We found that volumetric compression has a significant effect on the energetics of vacancies. The formation energy of mono-vacancy decreases with increasing compression monotonically. The $\langle 111 \rangle$ di-vacancies experience a binding-repelling transition when volumetric compression exceeds 13.2%. On the other hand, uniaxial deformation has weaker influence on the formation and binding energies. However, this type of deformation distinguishes $\langle 001 \rangle$ di-vacancies: those which are parallel to the strain have larger (smaller) binding energies than those perpendicular ones under compression (expansion). Our results indicate that external strain field is a key factor to modulate the concentration of vacancy and/or vacancy clusters in α -Fe.

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