

Synergistic Insights into the Tungsten-Tantalum-Vacancy System: A DFT-CE Study

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ABSTRACT

Tungsten (W) is a primary focus for applications facing plasma due to its high melting temperature; however, its brittleness poses notable challenges. To overcome this, exploration into W-based multi-component alloys is undertaken [1], with a specific emphasis on defect studies, including vacancies and interstitials. The determination of a new material's stable structure is crucial, and phase diagrams play a pivotal role. Consequently, Cluster Expansion (CE) serves as a link between first-principles energy methods and Monte Carlo simulations for the computation of phase diagrams. As the formation energy (E_f) of alloys (and thus the phase diagram) is contingent upon the local arrangement of different atoms around vacant sites, mono-vacancies are treated as an additional 'chemical' component in the W-Ta alloy. This treatment results in mapping the alloy onto a ternary system (W, Ta, Vacancy), enhancing the comprehension of vacancy concentration as a function of alloy composition, as demonstrated in the calculated W-Ta-Vacancy (WTaVac) phase diagram.

Concurrently, an examination of density functional theory (DFT) calculations during the creation of a mono-vacancy in W-Ta alloy of varying sizes indicates that the bond between Ta and W is robust. Creating a vacancy of a specific species becomes challenging when neighboring atoms are of different natures, implying a strong Ta-W bond. An analysis of bond stiffness versus bond length further suggests enhanced W-Ta bonding.

The outcomes of Monte Carlo (MC) simulations reveal vacancy clustering, with Ta atoms predominantly surrounding the vacancy clusters. This observation aligns with DFT calculations, where lower formation energies are noted for cases where Ta surrounds the vacancies compared to scenarios where vacancies have W atoms as their first near neighbors.

In conclusion, these findings suggest that vacancies induce partial segregation in alloys, potentially influencing their mechanical properties.

References

- [1] O. El-Atwani et al., *Sci. Adv.*, **5**, eaav2002 (2019).