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Miscibility gap in tungsten-based alloys

Our motivation is based on the fact, whether the pure tungsten is suitable alone for the first wall application of the fusion reactor, or it is better to be alloyed with elements that can increase the desired properties at elevated temperatures (e.g. oxidation resistance).
In this work we establish an approach to model miscibility gaps of alloys using statistical physics, lattice dynamics from first-principles calculations. We carefully calculate the entropy to include all processes introducing disorder to the system, i.e., combining the electronic, phononic, and configuration entropies. Furthermore we present our algorithm for generating Special Quasirandom Structures. We model the miscibility gap in tungsten - chromium and tungsten - molybdenum systems, obtaining the agreement with the experimental data. Furthermore, we propose an enhancement for the tungsten-chromium $W_{70}Cr_{30}$ alloy with tantalum and hafnium, leading to the modified stabilization temperatures (T_S), where the solid solution is miscible. The work was published in Refs. [1,2].

References:
1. A.P. Kadzielawa, D. Legut, International Journal of Refractory Metals and Hard Materials 115 (2023) 106272.
2. J. Veverka, M. Vilemova, F. Lukac, A.P. Kadzielawa, D. Legut, K. Vontorova, J. Kozlik, T. Chraska, Journal of Nuclear Materials 576 (2023) 154288.

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