A high-throughput approach to computational materials design: tungsten alloys for nuclear fusion reactors

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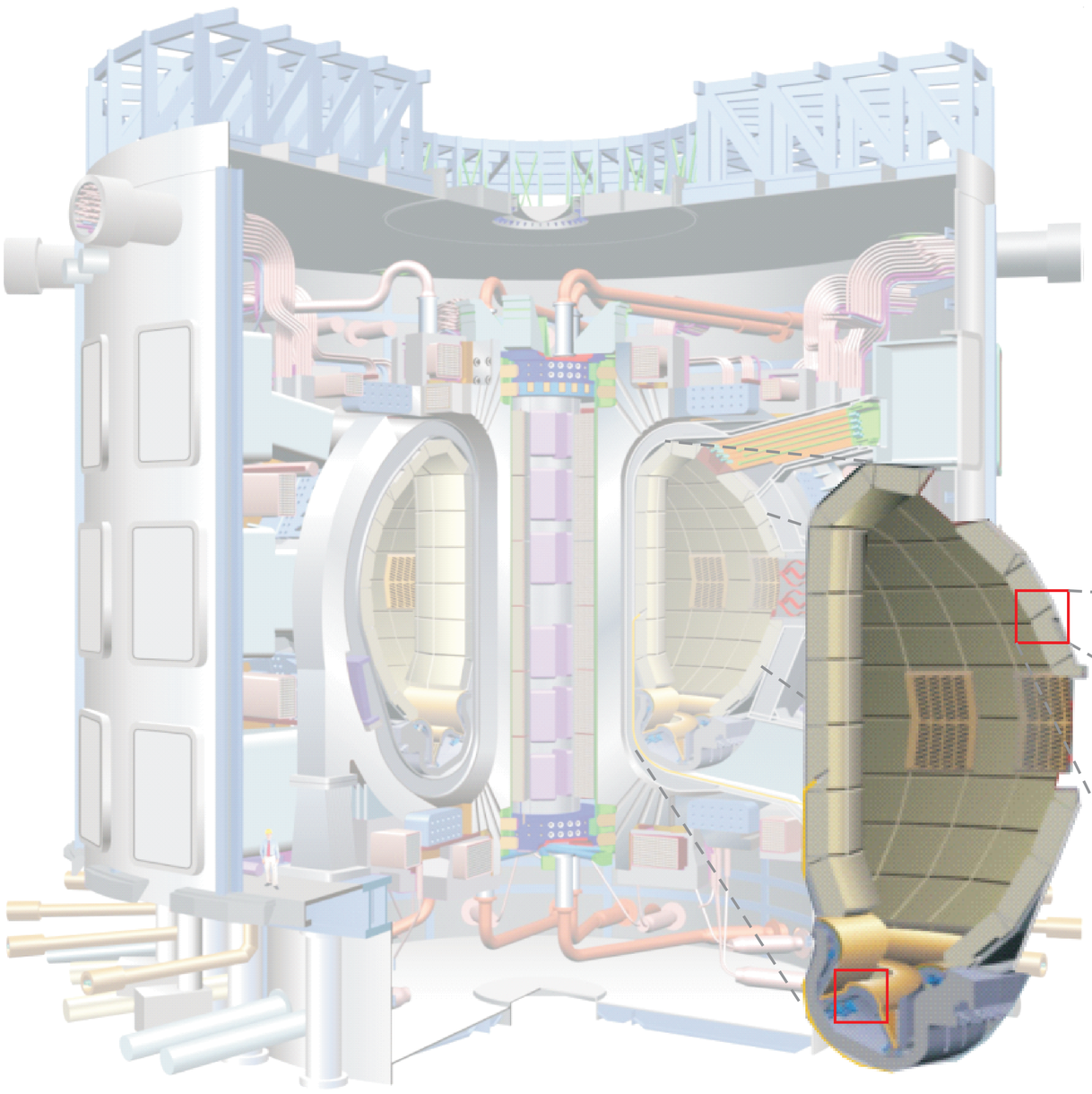
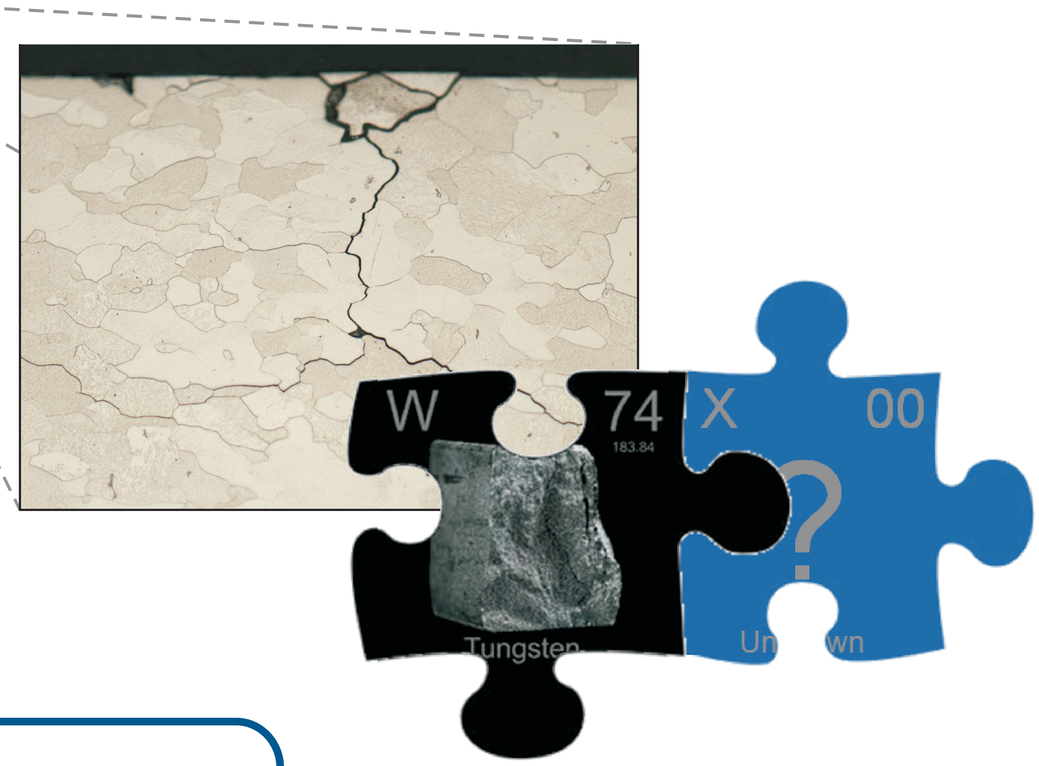


Introduction

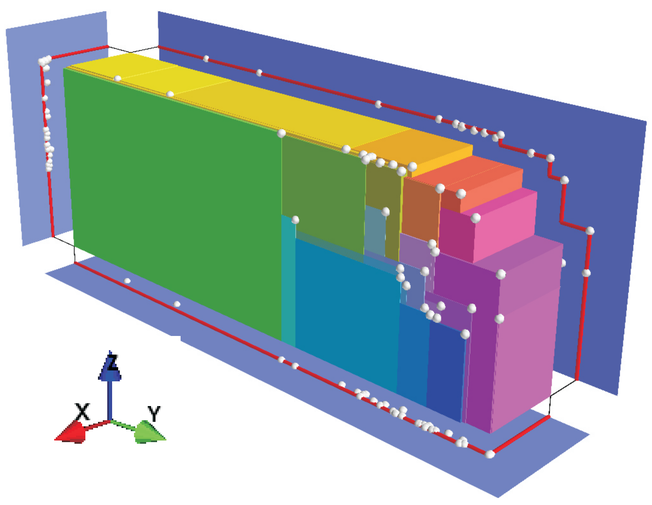
Nuclear fusion offers a sustainable answer to the world's increasing energy demands. However, there is still much work to be done before it can be applied commercially. ITER, which is currently being built in the south of France, will be the first reactor producing more power than it requires. Its successor, DEMO, will be the prototype for a real commercial plant. To address the harsh conditions in the interior of this machine, its inner components will mainly be made out of tungsten, which has a good high-temperature resistance (low thermal expansion, high melting temperature, ...) and behaves well under neutron irradiation.

Unfortunately, tungsten is brittle at room temperature, which makes it hard to process and which compromises the stability of the reactor wall during operation. Alloying tungsten with other elements might solve this problem. A (computational) screening helps identifying the best options.



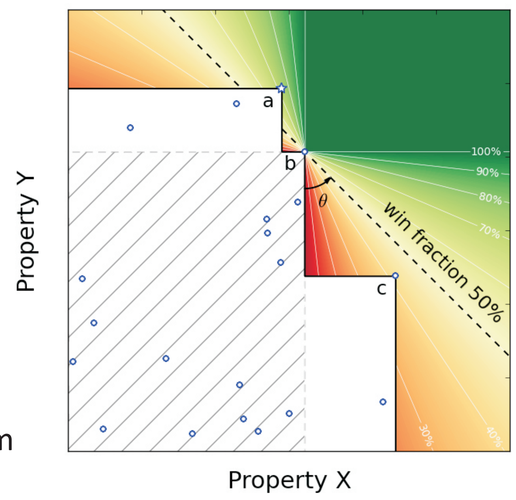
Multicriterion optimization

An optimal tungsten alloy improves the ductility of pure tungsten (y), while maintaining its other high-temperature advantages (x) and (relatively) low price (z). When simultaneously optimizing these objectives, the 'best' solutions form the so-called Pareto set. In 3D they represent a skyline over the data set.



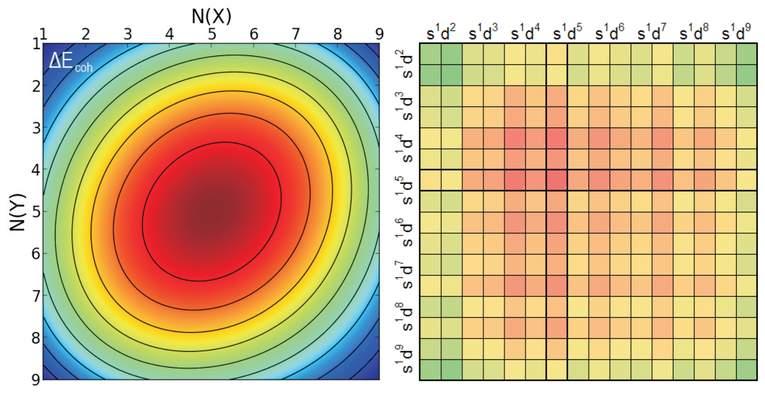
Beyond the Pareto set

For design purposes, the Pareto set is often still too large. To retain only the most promising materials, we defined the minimum win fraction (mwf), which allows ranking the Pareto compounds. Materials with a high mwf perform significantly better for most objectives and are only slightly worse for the rest.



Trends and deviations

Not only the best materials are of interest, but also the trends within the data set. These follow from the unsaturated, covalent-like character of the d bonds in transition metals (e.g. ΔE_{coh}; left: tight binding, right: DFT-PBE).



Outliers from the trends are also very valuable, as they arise from unexpected physical phenomena, which may render a material more suitable for the application at hand.

Application to the tungsten ternaries

We simultaneously minimize the thermal expansion coefficient, maximize one of four ductility predictors, and minimize the price from a database with ab initio calculated properties of 210 bcc ternary tungsten alloys $W_{30}XY$ (X and Y are 4d and 5d transition metals). We only inspect the energetically most favourable configuration of the two dopants within the 32-atom unit cell. Averaging the mwf over all four ductility predictors (C_{12}-C_{44}, B/G, C_{44}, $Gb^2/2$), yields $W_{30}ZrAg$ as the best option.

<mwf>	compound	<mwf>	compound	<mwf>	compound
38.3%	$W_{30}ZrAg$	16.1%	$W_{30}Ta_2$	12.7%	$W_{30}CdLu$
19.8%	$W_{30}Hg_2$	15.4%	$W_{30}Lu_2$	12.3%	$W_{31}Zr$
18.0%	$W_{30}AgHf$	13.4%	$W_{30}PdTa$	... 45 more Pareto ...	

Conclusion

By applying the concepts of Pareto optimality and the minimum win fraction to the computational design of fusion materials, a small set of promising candidates was identified. These can be further investigated experimentally.

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