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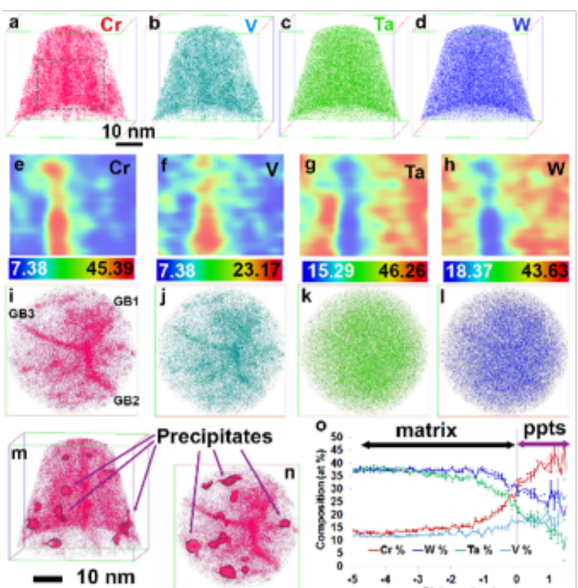
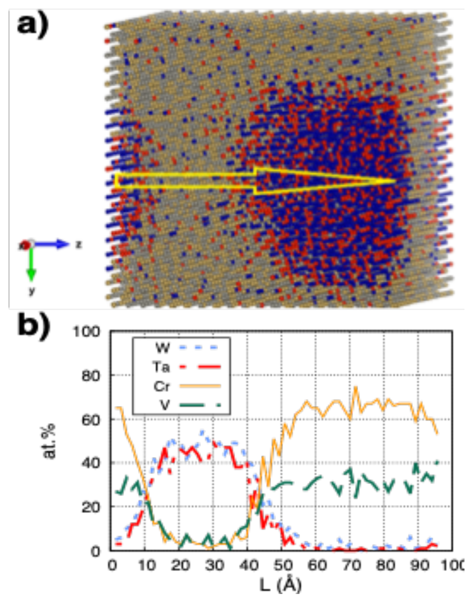
Outstanding Radiation Resistance of Tungsten-based High Entropy Alloys

A new tungsten-based alloy can withstand unprecedented amounts of radiation without damage. Essential for extreme irradiation environments such as the interiors of magnetic fusion reactors, previously explored materials have thus far been hobbled by weakness against fracture, but this new alloy seems to defeat that problem.





Left: The 3D distribution of Cr, V, Ta and W in the 8 dpa irradiated high-entropy alloy with 3 MeV Cu^+ at 1050 K revealed by atom probe tomography (APT) is shown in (a) to (d), respectively. 2D compositional maps of Cr, V, Ta and W using a 25x1x20nm slice of APT data is shown in (e) to (h) where the color scale bars below each figure denotes concentration values for each element. The top down view of the APT result showing the location of three distinct grain boundaries captured by APT as well as corresponding elemental segregation is shown in (i-l). (m) shows the side view of reconstruction with 25 at % Cr isocomposition surface showing Cr-V rich precipitates inside grains and the top down view is shown in (n). The compositional partitioning between the precipitate and matrix is shown in (o).

Right: Theoretical predictions of the atomic configurations. (a) Atomic configuration in a $W_{38}Ta_{36}Cr_{15}V_{11}$ alloys at T=1000K after canonical Monte Carlo simulations. (b) Average concentration profile of each element along the [001] direction.

The Science

A body-centered cubic W-based refractory high entropy alloy with outstanding radiation resistance has been developed. The alloy was grown as thin films showing a bimodal grain size distribution in the nanocrystalline and ultrafine regimes and a unique 4 nm lamella-like structure revealed by atom probe tomography (APT). Transmission electron microscopy (TEM) and X-ray diffraction show certain black spots appearing after thermal annealing at elevated temperatures. TEM and APT analysis correlated the black spots with second-phase particles rich in Cr and V. No sign of irradiation-created dislocation loops, even after 8 dpa, was observed. Furthermore, nanomechanical testing shows a large hardness of 14 GPa in the as-deposited samples, with near negligible irradiation hardening. Theoretical modeling combining *ab initio* and Monte Carlo techniques predicts the formation of Cr and V rich second phase particles and points at equal mobilities of point defects as the origin of the exceptional radiation tolerance.

The Impact

Key components in magnetic fusion reactors, such as the divertor or the plasma-facing materials (PFMs), are required to have stringent properties including low activation, high melting point, good thermo-mechanical properties, low sputter erosion and low tritium retention/co-deposition. They must operate at high temperature ($\geq$ 1000 K) for long durations ($> 10^7$ s), without failure or extensive erosion while exposed to large plasma heat and an intense mixture of ionized and energetic neutral species of hydrogen isotopes (D, T), He ash (fluxes $> 10^{24}$ $m^{-2}s^{-1}$) and neutrons. Current materials fail to withstand such harsh conditions, and therefore, the development of new material systems is paramount in order to enable fusion as a viable energy source.

Research Details

Nanocrystalline W-Ta-Cr-V was prepared via magnetron sputtering deposition from pure metal targets. In-situ TEM/irradiation was performed at RT and 1050 K using 1 MeV Kr^{++} and showed no sign of loop formation. Second phase precipitation of Cr-rich particles occurred as confirmed via Atom Probe Tomography. Nanoindentation showed small increase in hardness after thermal annealing and irradiation. A cluster expansion method was used to predict configurational energies fitted to DFT data, which coupled with Monte Carlo simulations accurately predicted the experimental results.

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Publications

Outstanding radiation resistance of tungsten-based high-entropy alloys, Science Advances, DOI 10.1126/sciadv.aav2002, O. El-Atwani, N. Li, M. Li, A. Devaraj, J. K. S. Baldwin, M. M. Schneider, D. Sobieraj, J. S. Wrobel, D. D. Nguyen-Manh, S. A. Maloy, and E. Martinez.

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