Dislocation core structures and slip planes in W alloys

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1. Introduction

Tungsten and tungsten alloys are promising structural materials for fusion-power-plant application [1], largely due to their excellent physical properties. However, a brittle to ductile transition above the room temperature seriously limits the formability of this materials and its resistance to mechanical load during the operation temperature range. Re alloying is known to have a ductilizing effect in VIA group metals (Cr, Mo, W), but the underline mechanism is still not clear. The ½<111> screw dislocation is believed to be the controlling factor for the plastic behavior in these systems [2], therefore, it is of great importance to investigate the properties of the screw dislocation and its response to stresses in these systems.

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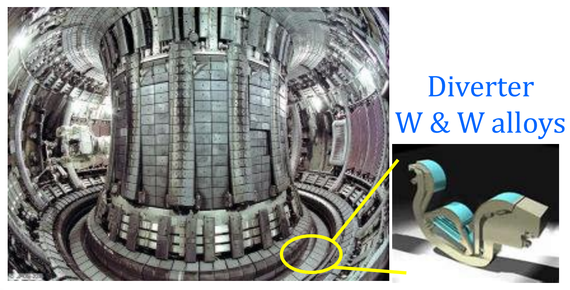
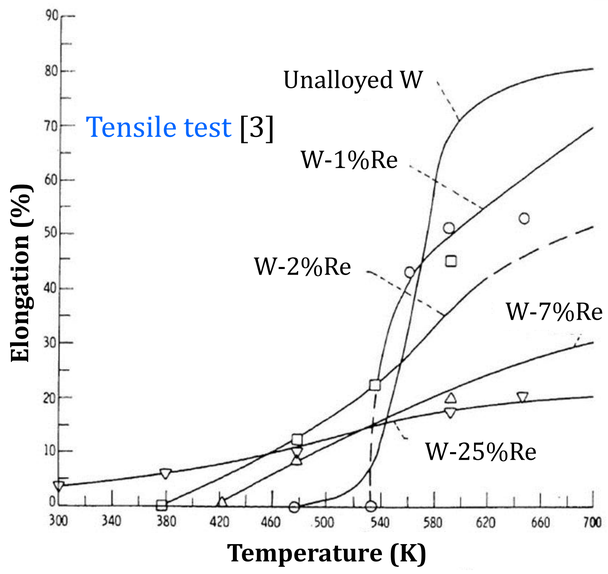
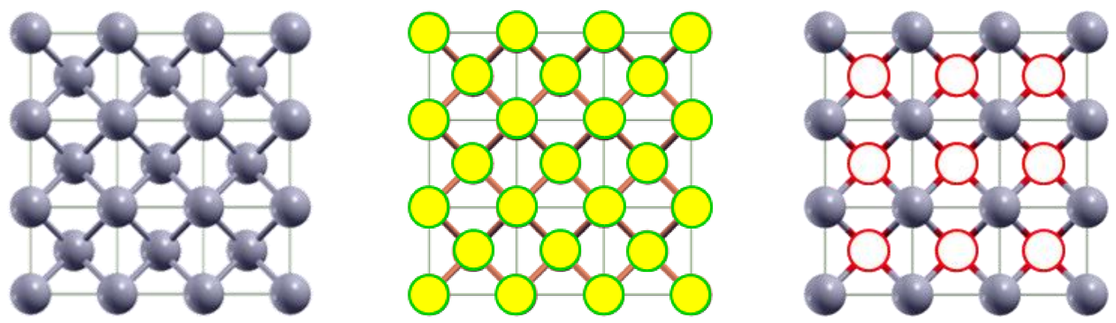




2. Methodology

All the calculations are performed within the framework of total-energy plane wave density-functional pseudo-potential approach using Quantum-ESPRESSO [4] and VASP code [5]. The Perdew-Burke-Ernzerhof exchange-correlation function was used throughout this work. For alloy simulation both the virtual crystal approximation (VCA) [6] and the normal supercell (SC) calculations are performed to obtain reliable results. In the VCA calculations an effective type of atom with intermediate nuclear and electronic charge is always used to construct the same lattice structure as the pure W phase, see figure below. While in the SC calculations a certain amount of W atoms are substituted by alloying elements at specific atomic positions.



(a) Pure W (b) VCA (c) SC

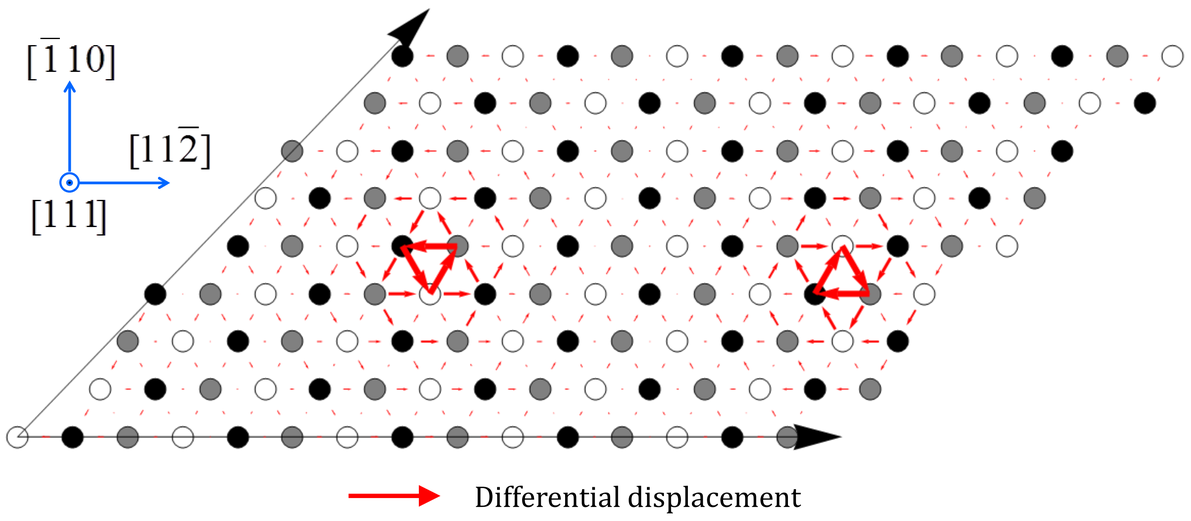
These two different types of calculation complement each other as the VCA calculation provides an average over many configurations, while the SC calculation provides the result for a specific alloying distribution.

3. Dislocation dipole approach

Two screw dislocations with anti-parallel burgers vector are insert in the unit cell according to linear elasticity. The displacement field is assigned by equation:

$$u_z(x,y) = \sum_i b_z \frac{\theta_i}{2\pi}$$

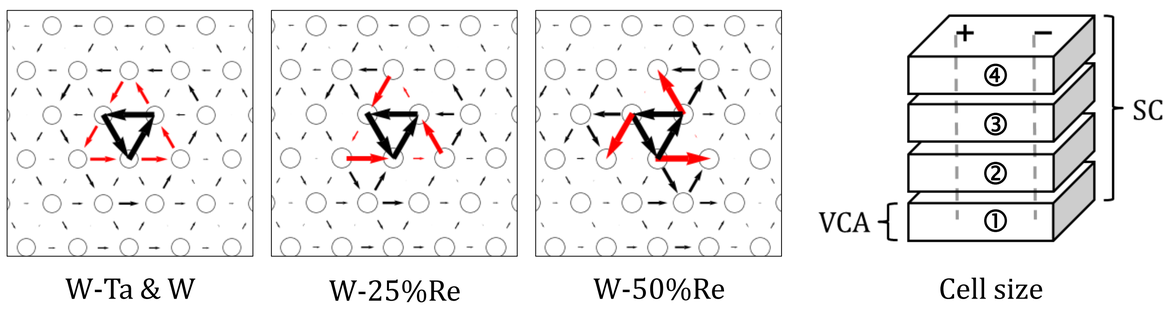
where θ_i is the angle of the vector connecting the point (x, y) with the dislocation center i.



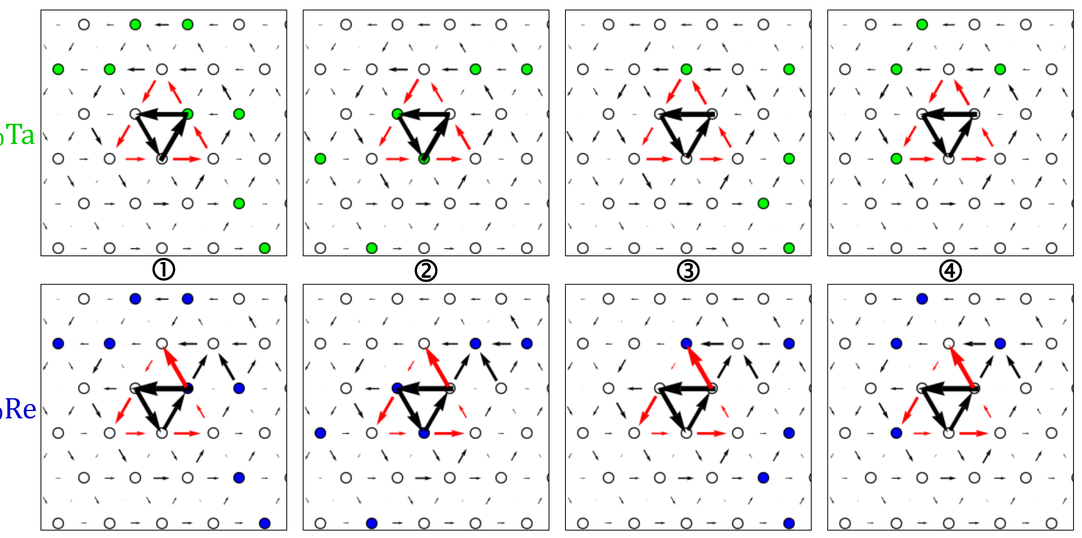
Dislocation dipole on the (111) surface represented by the differential displacement map. Atoms in three successive (111) planes are presented by white, gray, and black disks.

4. Dislocation core symmetry

A. Virtual crystal approximation calculations



B. Supercell calculations

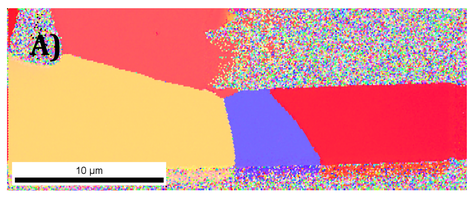


5. Slip planes

Modifying the cell vector $\vec{a}_2$ to $\vec{a}_2' = \vec{a}_2 + \epsilon_{[111]}$ as shown in the lower figure induces the Peach-Köhler force along $[11\bar{2}]$ and drives the dislocation to a neighboring triangle site, passing the high energy hard core state in between, when the stress is higher than the critical peierls stress.

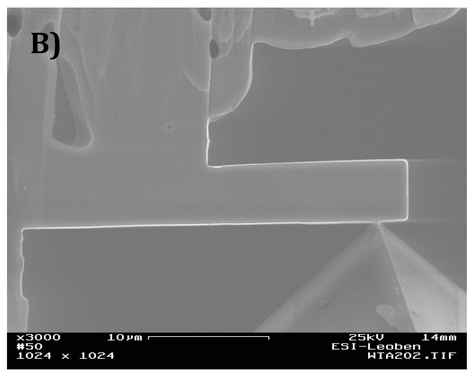
6. Experimental measurement

A) Crystal orientation map (Inverse Pole Figure map, IPF) from EBSD of a WTa. B) shows an SE-image of the experimental set-up for the same cantilever prior to in-situ-loading with a cube corner indenter.



Dimensions of cantilevers made of various tungsten-based materials and correspondent slip planes.

Material	Width W [µm]	Thinkness B [µm]	Bending length [µm]	Slip plane
W	5.7	6.0	26.3	{110}
W-24%Ta	4.6	8.6	17.5	{110}
W-24%Ta	4.9	4.5	14.0	{110}
W-26%Re	4.9	6.1	23.1	{112} {123}



7. Conclusion

Using density-functional theory approach the ½<111> screw dislocations in W alloys are investigated. It is found that Re alloying leads to the transition of symmetric core to asymmetric core in W, The symmetric core slips in {110} plane driving by the Peach-Köhler force, while the asymmetric core slips in a zig-zag manner, resulting in the general slip plane of {112}. The measurements of the slip traces on the micro-cantilever after bending tests provide good consistent results with the calculations for the preferred slip planes in W-Ta and W-Re alloys. Changing the slip plane from {110} to {112} increases the number of possible slip system and facilitates the mobility of the screw dislocations.

8. References

[1] S. J. Zinkle, Fusion Engineering and Design 74, (2005) 31.
[2] P. B. Hirsch, 5th International Conference on Cystallography, Cambridge University Press, Cambridge, 1960, p.1.
[3] P. L. Raffo, J. Less-Common Metals 17 (1969) 133.
[4] P. Giannozzi, et. al. J Phys.: Condens. Matter 21 (2009) 395502.
[5] G. Kresse, J. Hafner, Phys Rev. B 47 (1993) 558.
[6] L. Nordheim, Annalen Der Physik 9, (1931) 607.

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