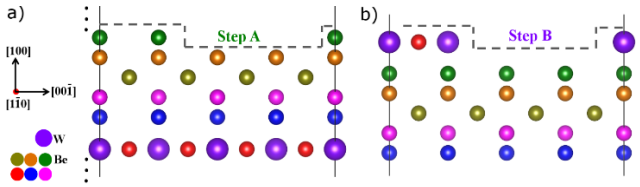
Beryllium, Tungsten and the Alloys Be_2W and $Be_{12}W$: Surface Properties from Density Functional Theory Calculations

Lei Chen, Alexander Kaiser, Ivan Sukuba and Michael Probst
Institute of Ion Physics and Applied Physics, University of Innsbruck, 6020 Innsbruck, Austria

Abstract

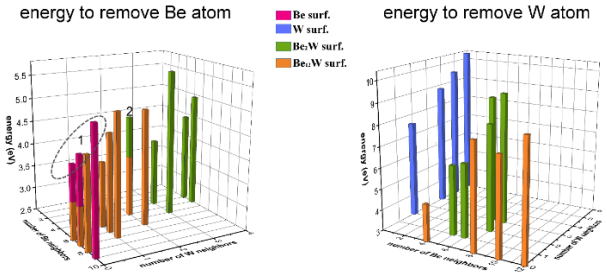
Energies for binding, adsorption and displacement of the surface atoms Be and W of Be/W alloys with several major orientations have been obtained from density functional theory calculations. Motivation for this work arises from the material-science aspects of the fusion reactor ITER in which several components will be made from Be and W. The analysis of adatom formation on viable surfaces can predict the adsorption and step formation and finally the degradation processes that will occur in a material facing a hot plasma.

The calculations were performed with VASP. Stoichiometric systems were constructed as slabs with surface terminations in the (110) or (111) planes. The thickness of the vacuum, or specifically the length of vacuum along the direction perpendicular to the slab surfaces was chosen to be 8 Å. Kohn-Sham density functional theory (DFT) was used to predict the electronic ground state energy and to optimize the structures. A plane-wave (PW) basis set with a kinetic cutoff energy of 550 eV was employed. The Projector Augmented Wave (PAW) method and the PBE exchange-correlation functional describe the core and valence electrons. Standard PAW potentials for W (with six valence electrons) and Be (with two valence electrons) were used. The picture below illustrates two supercells with two different steps.



Side view ($\vec{a}\vec{c}$ projection) of six topmost layers in $Be_{12}W$ supercell. Steps A and B were generated by adding half-slab of atoms on surface terminations Slab B and A (shown in **Fig. 2**), respectively.

We find that the number and kind of neighbors and the a kind of the atom determine the evaporation energy of a surface atom but that the correlation is complicated. In the following picture our results are summarized.



Energy needed to remove one Be(W) atom from Be, W, Be_2W and $Be_{12}W$ surface systems against the number of the nearest Be`(W) neighbors for the removed atom.

In words, W neighbors significantly influence energies to remove Be atoms. In the absence of thse, Be atoms of $Be_{12}W$ surface systems are less strongly bond than for pure Be. The reason is that Be atoms are more close-packed in pure Be than in $Be_{12}W$, leading to shorter distances between Be atoms. The energies to remove W atoms range from 4.77 eV for the atom with four Be NNs in Be_{12} to 10.27 eV for the atom with six W NNs in pure W. Similarly, the number of W neighbors exerts influences these energies. Generally, the energies go up with the W content in the material: W atoms of pure W surface systems are more stable than in Be_2W, and those are more stable than in $Be_{12}W$.