# Surface effects on the displacement energy of tungsten

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## Introduction

Tungsten has important application in design of the fusion reactor walls facing plasma, showing low sputtering rate and low hydrogen retention rate.

- Properties of surface layers facing plasma are currently intensively studied to identify the limitations to its use in the fusion reactors.

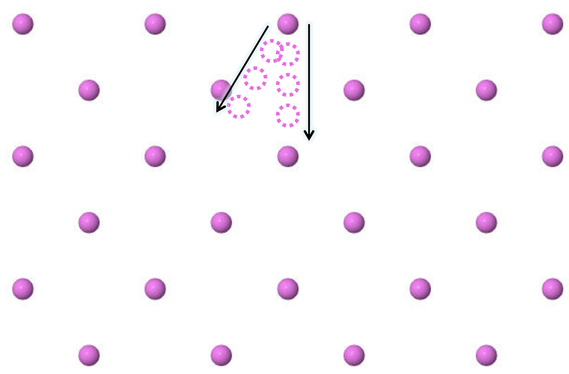
Using classical molecular dynamics (LAMMPS), we calculated, in the surface layers of tungsten bcc crystal at 300 K:

- The vacancy creation energies ($E_V$)
- The displacement energies ($E_D$) for impact along various crystal-lographic directions

## Methods

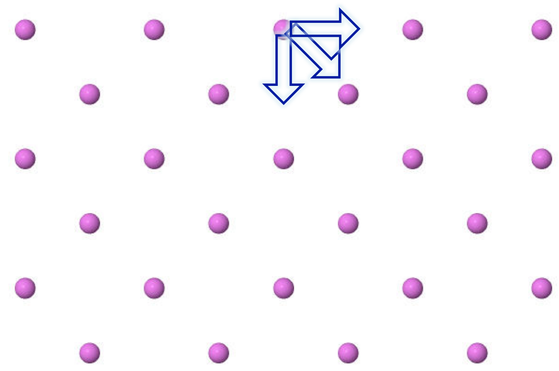
### Vacancy creation energy:

1. An A atom is moved from its lattice position
2. Relax other atoms
3. Calculate the potential energy of atom A at various displacements from its lattice position
4. Find the size of energy barrier = minimum vacancy creation energy.



### Atom displacement energy:

1. Set initial velocities of atom A in corresponding to various impact energies in one of the crystallographic directions
2. Induce impact cascade and follow its evolution until stable state is achieved
3. Find the minimum impact energy that can result in stable defect(s).



## Vacancy creation energy

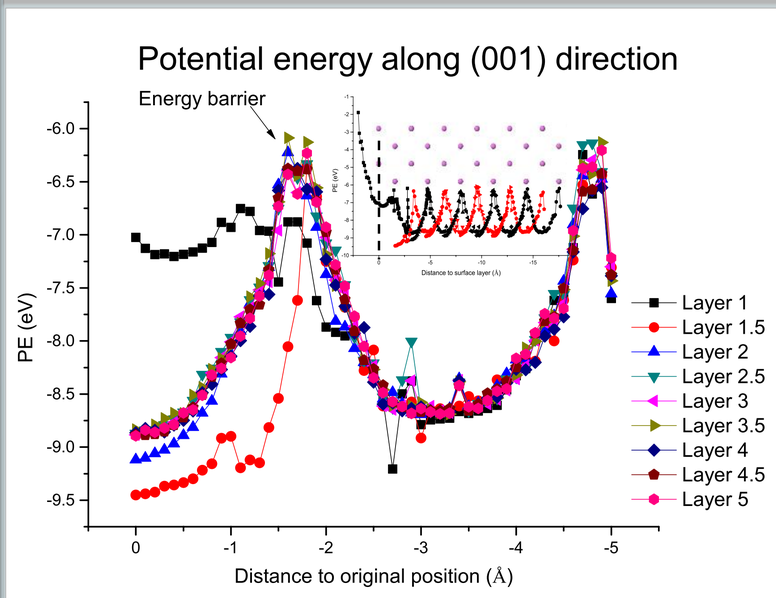



**Fig.1** Potential energy along (001) direction for the first 5 tungsten layers counted from the surface. Inset is the shifted figure with distance relative to surface atom layer. The energy barrier is the difference between first peak potential energy (PE) value and PE value at lattice position.

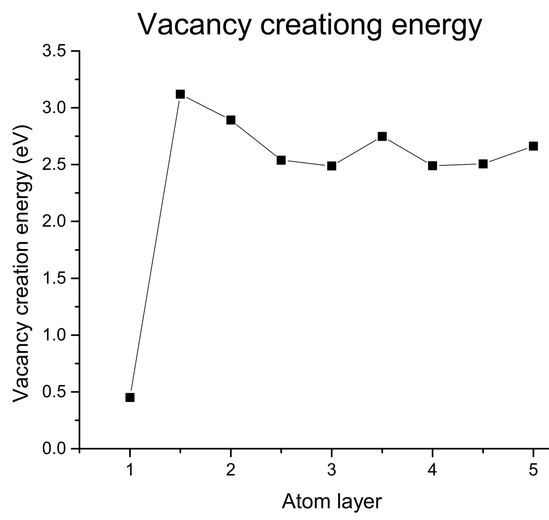



**Fig.2** Vacancy creation energy on different atom layers, derived from Fig.1. Bulk value of 2.63eV, evaluated by averaging all $E_V$ values after 3rd layer, is close to Henkelman's result (2.699eV), [1] but is a little lower than experimental result from Kraftmakher and Strelkov (3.14eV). [2]

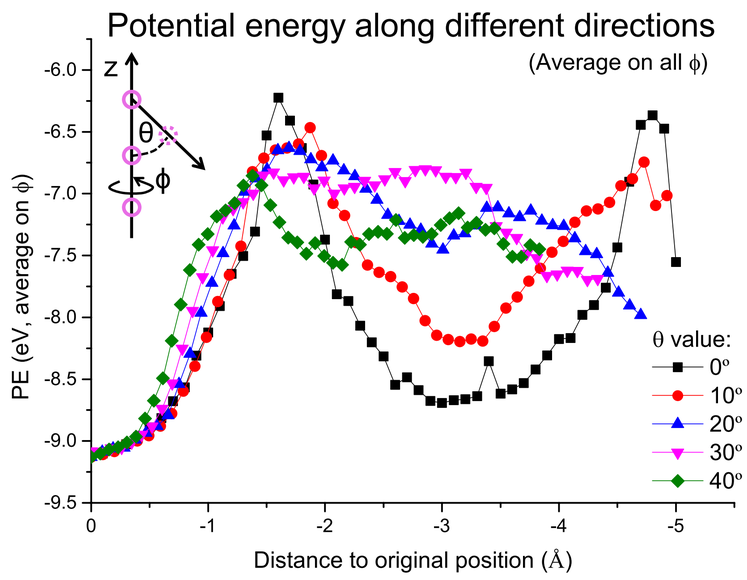



**Fig.3** Potential energy of 2nd atom layer along different directions. The value of each point is an average over all values of different ϕ. The vacancy creation energy is decreasing with the increase of θ angle.

## Displacement Energy

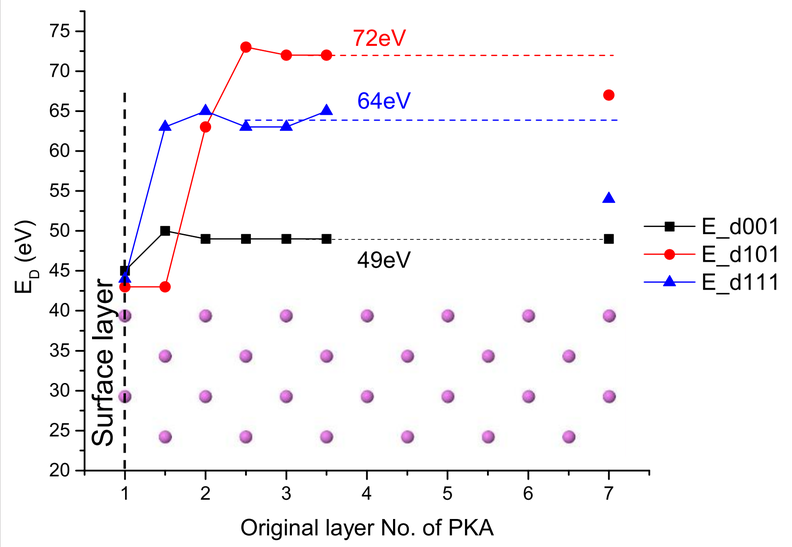



**Fig.4** Displacement energy of different atom layers for impact along (001) (101) and (111) directions. $E_D$ of 1st atom layer for all three directions are close to 44eV. As it gets to inner atom layer, $E_D$ first increases and finally reaches bulk value with a small decrease, which corresponds to the variation of $E_V$. The minimum $E_D$ value of 49eV is consistent with the experimental result of 42eV obtained by Maury. [3]

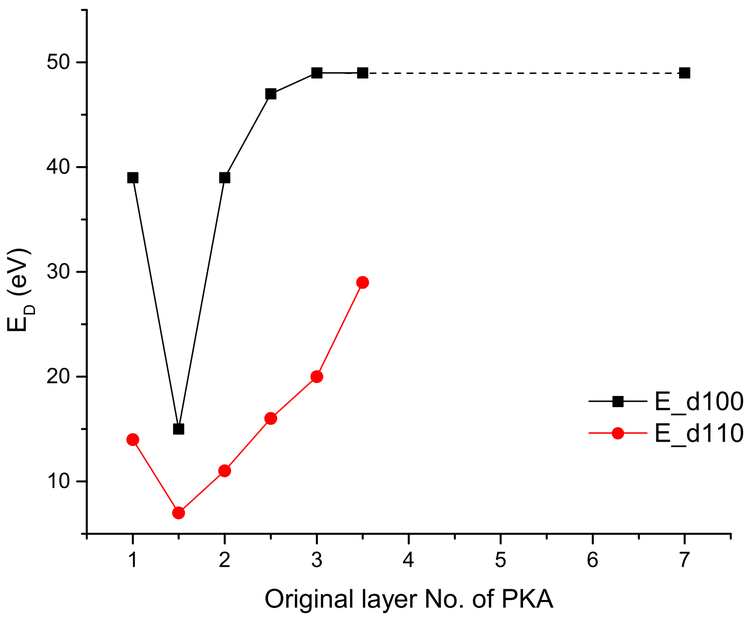



**Fig.5** Displacement energy of different atom layers for impact along (100) and (110) directions (parallel to the surface). Minima are observed for first intermediate atom layer (Layer 1.5), which can be explained by the easy knock-off of 1st layer atom by PKA. $E_D$ of (100) direction is the same with that of (001) direction, which is in the same family of direction. In (110) direction, $E_D$ was not displayed because defect cannot be observed for energy up to 150eV.

## References

1. http://theory.cm.utexas.edu/wiki/index.php/Tungsten_studies
2. Schultz, H. : Quenching of Vacancies in Tungsten. Lattice Defects in Quenched Metals. R. M. J. Cotterill, et al., eds., Academic Press, 1965, pp, 761-765.
3. F. Maury, M. Biget, P. Vajda, A. Lucasson, P. Lucasson, Rad. Eff. 38 (1978) 53.

## Conclusion

A molecular dynamics study with BOP potential is used to calculate the vacancy creation energy ($E_V$) and threshold displacement energy ($E_D$) of primary knock-on atoms, in the surface layers of tungsten bcc crystal lattice at 300 K and at various crystallographic directions. The vacancy creation energy of the first atom layer is only **1/5 of bulk value**. Depending on the direction, displacement energy $E_D$ is **10% to 75% smaller from the bulk value** at the first layer, interfacing vacuum, while it reaches close to the bulk value already at the third atomic layer.