Ab Initio Modeling of Point Defects and Gas Atoms in Beryllium

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Motivation

Beryllium is considered as the first wall armor material and as neutron multiplier for the blanket of fusion reactor. Radioactive hydrogen isotope T can be either implanted from plasma or generated through neutron induced nuclear reactions.

Retained tritium poses a potential safety and waste issue.

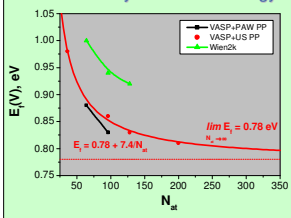
Modeling of tritium release from irradiated Be is indispensable for evaluation of the amount of retained T and extrapolation of the experimental results obtained using fission reactors to fusion irradiation conditions.

Simulation Method

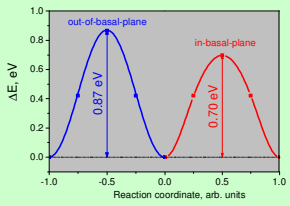
- Density functional theory based code VASP
- generalized gradient approximation (GGA-PW91)
- Supercells: 64-200 atoms
- Convergence test of cut-off energy and the number of k-points
  - ENCUT = 450 eV
  - 13x13x13 k-points
- Diffusion barriers were calculated using nudged elastic band (NEB) method

Vacancy and Self-Interstitials

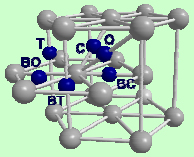
Vacancy Formation Energy



Vacancy Diffusion Anisotropy

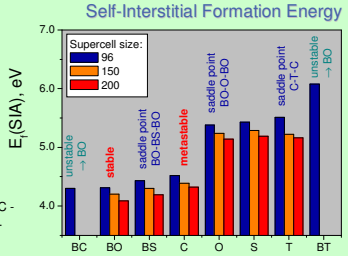


Self-Interstitial Positions



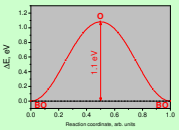
O-octahedral position, T-tetrahedral, BT and BO - basal tetrahedral and octahedral, C - crowdion, BC - basal crowdion, S -split dumbbell, BS - basal split.

Self-Interstitial Formation Energy

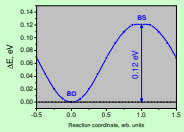


Self-Interstitial Migration Paths

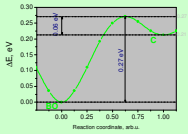
BO-O-BO: jump along c axis



BO-BS-BO: jump in basal plane

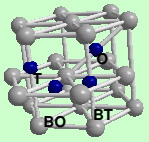


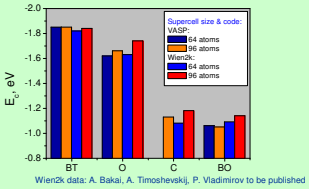
BO-C: jump out of basal plane



Hydrogen in Be

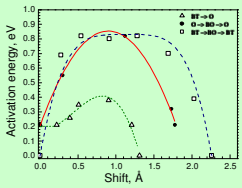
Interstitial Hydrogen





Wien2k data: A. Bakai, A. Timoshevskij, P. Vladimirov to be published

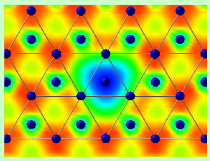
Interstitial Hydrogen Diffusion



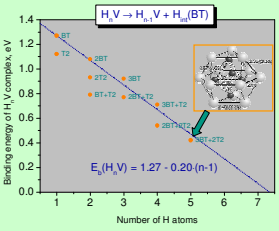
O → BT 0.16 eV
BT → O 0.38 eV
O → O 0.60 eV

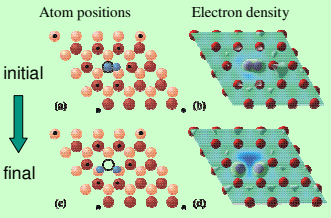
Effective migration energy: 0.38 eV
Exp. measured : 0.36 eV

Hydrogen in Vacancy



Electron density distribution around vacancy

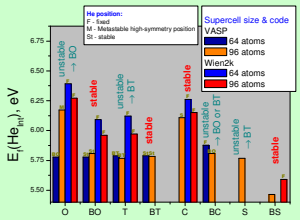




H_2 molecule is unstable inside vacancy

He-Interstitials and He in Vacancies

Interstitial He formation energies



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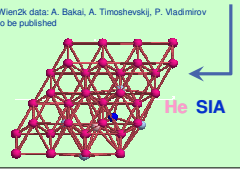


Interstitial He diffusion

Along c axis:

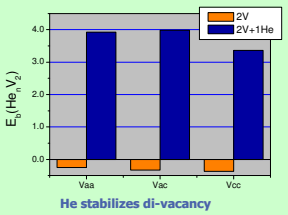
BO → O → BO E_m = 0.36 eV

In basal plane:

BO → BT E_m = 0.1 eV

C → O → C E_m = 0.12 eV

Binding energy of HeV_2



He stabilizes di-vacancy

Conclusions

- Di- and tri-vacancy clusters are unstable in Be, but are stabilized by gas atoms.
- DFT calculations correctly reproduce experimentally observed anisotropy of vacancy diffusion: 1.5 eV in basal and 1.67 eV out of basal plane.
- BO position is the most favorable for SIA in Be. C position is metastable. Other positions are unstable and usually represent saddle points along migration paths.
- SIA diffusion is anisotropic: 0.12 eV in basal plane and 0.27 eV out of it.
- BT position is the most favorable for the interstitial H. Effective migration energy is 0.38 eV in good agreement with exp. data (0.36 eV).
- Vacancy is an efficient trap for up to 5 H atoms: 0.4 - 1.27 eV.
- H_2 is unstable within a single vacancy. However, it is not excluded that it might be stable inside large vacancy clusters.
- Various He interstitial positions are stable: C, BO and BT, but the most favorable is basal split (BS) which relaxes to a kind of substitutional He – SIA cluster.
- Considered diffusion paths show anisotropic character of interstitial He diffusion: 0.1 eV in basal and 0.36 eV out of basal plane.

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