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# Simulation of hydrogen effect on equilibrium shape of gas bubbles in beryllium

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#### Abstract

In fusion environment hydrogen isotopes can be either produced inside beryllium bulk or adsorbed on beryllium surface. In the present work the effect of hydrogen surface concentration on the properties of five principal hexagonal close-packed beryllium surfaces (basal, prismatic type I and II, pyramidal type I and II) was studied by first-principle calculations. The configurations with high hydrogen coverage were studied for all considered surfaces. It was shown that the presence of adsorbed hydrogen atoms significantly changes the energy of all surfaces with except the prismatic type II surface. Influence of hydrogen surface concentration on the equilibrium shape of hydrogen covered bubbles was investigated by means of the Wulff polyhedron construction.

Keywords: beryllium, hydrogen, equilibrium shape of gas bubbles, simulation

#### 1. Introduction

Beryllium is very promising material for fusion energy applications due to its ability for neutron multiplication [1, 2]. The Helium Cooled Pebble Bed Blanket with beryllium pebbles is the advanced concept of the tritium breeding blanket for the future demonstration fusion reactor DEMO. In this concept lithium ceramic is used as tritium breeding material, while beryllium acts as neutron multiplier. High-energy fusion neutrons result in transmutation of beryllium atoms into betaradioactive tritium and helium and, as a consequence, to formation of gas bubbles and degradation of the material properties. Tritium is captured by vacancies and gas bubbles. Assessment of the radioactive inventory of tritium trapped inside beryllium pebbles is very important from the safety point of view during operation and for handling of the radioactive beryllium waste after the end-of-life of the blanket. On the other hand, the concept of ITER considers beryllium as plasma facing material for the first wall. Under such conditions interaction of hydrogen isotopes with beryllium surfaces is also unavoidable.

Experimental studies and *ab initio* calculations show that the presence of hydrogen atoms on beryllium surface leads to a considerable change of its properties. A significant interplanar relaxation of the outermost atomic layers accompanied by the change of the structural and energetic characteristics takes place [3, 4, 5, 6, 7, 8, 9, 10]. Note, that majority of the available first-principles studies consider mainly the basal and prismatic type I planes only [3, 4, 5, 6, 7, 11, 12, 13]. In order to investigate an equilibrium shape of gas filled bubbles it is necessary, however, to extend our knowledge about the energetics of the principal hcp surfaces with and without hydrogen.

For understanding of the presented results it is necessary to mention that: (i) hydrogen molecule undergoes dissociative adsorption on beryllium surface, (ii) hydrogen atoms can desorb from the surface only as a molecule, (iii) hydrogen atoms repel each other on the surface thus preventing their desorption from the surface until high hydrogen surface concentration is reached or the temperature is high enough to overcome desorption barrier, (iv) there exist upper limits for hydrogen concentrations on beryllium surfaces above which athermal desorption of hydrogen molecules occurs; these concentrations will be referred as maximum or 100% coverage below, (v) significant hydrogen surface concentration can be accumulated on the inner surface of helium bubbles which will result in notable changes of surface energies of various bubble facets and will lead to the change of the equilibrium gas bubble form.

Gas bubbles in beryllium are often formed after neutron irradiation at elevated temperatures (above 400-500° C). In this case both helium and tritium are produced due to nuclear transmutation. Small bubbles are usually faceted having a form of a hexagonal prism extended on basal plane. These bubbles are mainly filled with helium as far as about ten times more helium than tritium is produced in typical mixed spectrum nuclear reactor [14]. On the other hand, bubbles formed after annealing of hydrogen implanted beryllium at 400-600 °C have completely different shape [15].

The main goal of the present work is to study the effect of hydrogen surface concentration (coverage) on beryllium surface energies via first-principle calculations. The obtained results are used for construction of the equilibrium shape of bubbles covered with hydrogen and compared with experimental results obtained after neutron irradiation or hydrogen implantation.

# 2. Simulation methods

Static first-principles calculations were performed using the Vienna Ab initio Simulation Package (VASP) [16, 17]. The projector augmented wave potentials (PAW) were used to describe

the interactions between ions and electrons. The PAW potentials for beryllium (with two valence electrons) and hydrogen were taken from the VASP depository [18, 19]. The generalized gradient approximation (GGA) of Perdew and Wang [20] was employed to determine the exchange-correlation energy.

Hydrogen effects were studied for five principal close-packed beryllium surfaces: basal (0001), prismatic type I ( $1\overline{1}00$ ) and II  $(2\overline{1}\overline{1}0)$  as well as pyramidal type I  $(1\overline{1}01)$  and II  $(2\overline{1}\overline{1}2)$ . For the prismatic type I and pyramidal type I surfaces, which can be terminated in two possible ways, only the most energetically favorable "short" termination was considered. A vacuum gap of 17-23Å equivalent to four atomic layers and sufficient to avoid interaction between the top and the bottom of the simulation box due to periodic boundary conditions was used. During energy minimization both volume and shape of the simulation box were fixed, while no restrictions on the relaxation of atoms were imposed. The optimized lattice constants for pure beryllium were a = 2.265Å and c = 3.562Å. A Fermi broadening of 0.2 eV and the cut-off energy of the plane waves of 450 eV were chosen after extensive verification. The atomic structures were visualized using the Jmol program [21].

For surface energy calculations five different configurations with the free surface area large enough to avoid the interaction of the hydrogen atom with its periodic images were created (see Table 1). This imposes certain restrictions on the thickness of the slab, since the number of atoms should not be too large to get reasonable calculation times. For convenience of surface energy calculation hydrogen atoms in the initial configurations were placed symmetrically on both free surfaces at the most energetically favorable adsorption sites found for single hydrogen on otherwise hydrogen-free surface: hcp hollow site for basal plane; bridge site at the 'surface ridge' for prismatic type I and II as well as pyramidal type II planes; a middle of triangle formed by two beryllium atoms at the 'surface ridge' and one atom at the 'surface valley' (see [10] for details).

The surface energy of beryllium slab covered by n hydrogen atoms was defined as

$$E_s = \frac{1}{2S} (E_{total}^{\text{Be}+n\text{H}} - E_{total}^{\text{Be}} - nE_{ref}^{\text{H}}), \qquad (1)$$

where  $E_{total}^{\text{Be+nH}}$  is the total energy of the beryllium system with *n* hydrogen atoms;  $E_{total}^{\text{Be}}$  is the total energy of the hydrogen-free beryllium slab;  $E_{ref}^{\text{H}} = -3.3590$  eV is the energy per hydrogen atom in H<sub>2</sub> molecule; *S* is the surface area. Factor two in Eq. (1) corresponds to the fact that the slab has two surfaces with equivalent hydrogen configurations on both sides.

It should be noted that our *ab initio* molecular dynamics runs reveal that there is an upper limit for hydrogen coverage on (0001) surface of beryllium in equilibrium with molecular hydrogen gas phase above which hydrogen molecules cannot be adsorbed. For the basal surface this critical coverage corresponds to one hydrogen atom per beryllium surface atom (or equivalently one hydrogen per surface lattice unit cell). In order to determine the critical hydrogen occupations for other surfaces, the stability of configurations with increasing number of hydrogen atoms adsorbed was checked by performing static VASP relaxations. This procedure was performed by placing hydrogen at different adsorption sites for each of the five considered beryllium surfaces. Thus, the following maximum surface coverage per surface unit cell was obtained: one hydrogen atom on basal plane; two hydrogen atoms on prismatic type I, type II and pyramidal type I planes; four hydrogen atoms on pyramidal type II plane (see Table 1).

Knowledge of the surface energy for various close packed surfaces allows us to determine an equilibrium shape of a gas bubble by means of the Gibbs-Wulff construction [22]. This procedure consists in minimization of the total surface free energy. The Wulff theorem states that the distance from a polyhedron face to its center should be proportional to the surface energy of this face. The Wulff shape of bubble was determined by construction of Voronoi polyhedron according to this rule.

# 3. Results

## 3.1. Beryllium surfaces at monolayer hydrogen coverage

Configurations with 100% hydrogen (monolayer) coverage are shown in Figure 1. It was found that at high concentrations hydrogen prefers to have two-fold coordination with beryllium surface atoms in contrast to lower coverages where in half of the cases hydrogen is three-fold coordinated. Atop-like positions for hydrogen adsorption were not observed in our simulations.

At high coverage the bridge position turns into a stable adsorption site and is the most energetically favorable (see Fig. 1a), although at low coverage it corresponds to a saddle point between hcp and fcc adsorption sites [10]. At high coverage the hcp and fcc hollow sites do not correspond to the energy minima anymore. For example, the energy difference of the fcc and the bridge sites on the fully covered surface is 0.22 J/m<sup>2</sup>.

For prismatic type I plane the stable hydrogen sites are along the surface 'ridge' and 'valley' as illustrated in Fig. 1b. All hydrogen atoms are located at bridge positions.

For prismatic type II plane hydrogen atoms can be located at bridge positions along surface ridges and valleys as shown in Fig. 1c, which is similar to stable hydrogen sites of single atom. However, different hydrogen occupations of the  $3 \times 3$  surface results in quite different results: (i) the configuration with 3 hydrogen in the valleys and 6 on the ridges is stable, (ii) the configuration with 6 hydrogen in the valleys and 3 on the ridges results in formation of Be-H chains and surface disordering, while (iii) the configuration with 6 hydrogen in the valleys and 6 on the ridges reveals formation of BeH<sub>2</sub> chains detaching from the surface during relaxation.

For pyramidal type I plane the half of hydrogen atoms are located at the bridge sites, while the other half is close to be three-coordinated with beryllium surface atoms (see Fig. 1d). Note that both stable sites found for single hydrogen atom are three-coordinated [10].

For pyramidal type II plane all stable adsorption sites are bridge-like positions. Figure 1e demonstrates that there is a certain asymmetry in the position of hydrogen atoms along the surface valley suggesting that the energy difference between them supposed to be insignificant.

Table 1: Surface energies of hydrogen free and 100% H-covered principal close-packed beryllium surfaces.  $N_{\text{Be}}$  is the number of beryllium atoms in the slab.  $N_{\text{H}}^{max}$  is the number of hydrogen atoms corresponding to 100% of coverage. The fourth column indicates the number of beryllium atomic layers in the simulated slab.  $E_s^{0\%}$  and  $E_s^{100\%}$  are the energies (J/m<sup>2</sup>) of hydrogen-free and 100% covered beryllium surfaces, respectively.

Surface	cell size	$N_{\mathrm{Be}}$	Be layers	$N_{ m H}^{max}$	k-points	$E_s^{0\%}$	$E_s^{100\%}$	
(0001)	$3 \times 3 \times 4$	72	8	9	$18 \times 18 \times 5$	1.71	1.64	
(1100)	$2 \times 3 \times 6$	72	12	12	$14 \times 15 \times 5$	1.80	1.53	
$(2\bar{1}\bar{1}0)$	$3 \times 3 \times 3$	108	6	18	$9 \times 10 \times 8$	2.02	1.88	
(1101)	$3 \times 2 \times 6$	72	12	12	$15 \times 12 \times 5$	1.83	1.08	
(2112)	$3 \times 2 \times 4$	96	8	24	$11 \times 15 \times 8$	2.40	0.76	

#### 3.2. Beryllium surface energy vs. hydrogen coverage

The effect of consecutive addition of hydrogen atoms on surface energies of various orientations is presented in Fig. 2. Generally, the surface energy first reduces, reaches a minimum and then raises with the increase of hydrogen coverage. Thus, from a certain point, which is different for different beryllium surfaces, further hydrogen adsorption is energetically unfavorable. The energy of all considered beryllium surfaces covered with hydrogen atoms is always smaller than that of the corresponding clean surface. The energies of prismatic type I and pyramidal type I surfaces at zero coverage are almost equal, but they differ by 0.4 J/m<sup>2</sup> in the case of monolayer coverage. The presence of hydrogen changes drastically the energy of pyramidal type II surface from 2.4 down to  $0.8 \text{ J/m}^2$ . In this way the most unfavorable surface turns out to be the most favorable after hydrogenation. On the other hand, the prismatic type II surface is not very sensitive to the presence of adsorbed hydrogen showing the surface energy changes in the range of 0.2 J/m<sup>2</sup> (10%). It is interesting to note that when the coverage exceeds 40%, the pyramidal type II surface becomes the most energetically favorable one (see Fig. 2), while the energy of basal surface is  $0.4-0.8 \text{ J/m}^2$  higher.

# 3.3. Equilibrium shape of hydrogen covered bubbles in beryllium

As a first approximation Wulff construction was performed assuming that hydrogen concentration is the same for different beryllium surfaces, although this assumption might be not necessarily valid. Figure 3 illustrates the computed equilibrium shapes of a bubble in hcp beryllium crystal without hydrogen (0% of coverage), which is composed mainly of basal, prismatic type I and pyramidal type I faces. Similar equilibrium shapes were obtained for other hcp materials [32, 24, 25, 26]. The only difference from the previous works is the presence of a small fraction of prismatic type II face (magenta) which cuts an edge formed between two adjacent prismatic type I faces. Since hydrogen considerably decreases the beryllium surface energy, the change of equilibrium shape of bubbles is expected with the increase of hydrogen coverage. Indeed, a full disappearance of prismatic type II, a slight decrease of the area of prismatic type I and an increase of the fraction of pyramidal type I facets are seen at 17% of coverage. Further increase of hydrogen concentration leads to a significant increase of the area of pyramidal type II facets. At 46% of coverage the bubble is faceted with

basal and pyramidal type II planes, while at monolayer coverage only pyramidal type II facets are present.

#### 4. Discussion

As we learned for the basal surface, the stable hydrogen adsorption sites at high coverage can noticeably differ from those with lower coverage. At high coverage, in the majority of the cases, hydrogen atoms prefer to occupy bridge sites and to be two-fold coordinated (see Fig. 1). A number of early *ab initio* simulations [27, 28] have revealed that on the basal plane the bridge position above the middle of the Be–Be bond is a stable adsorption site for one hydrogen atom in the smallest  $1 \times 1$ simulation cell. Our study confirmed that these results were not artifacts related to the small size of the simulation cells common at that time: stable bridge adsorption sites were repeatedly reproduced with larger simulation cells at high hydrogen coverages.

More recent study [29] of Be(0001) surface reported higher hydrogen coverage than that found in this work suggesting that  $3 \times 3$  cell, which includes 9 beryllium surface atoms, is completely covered, when 12 hydrogen atoms are present. As can be seen from the Fig. 3c therein most of the hydrogen atoms are two-fold coordinated and form a kind of disordered Be-H chains on the surface. As was mentioned earlier, our attempt to to put two hydrogen atoms per one beryllium (corresponds to 18 H per 9 Be) on the basal surface ended with athermal desorption of several hydrogen molecules, while no desorption was observed with one hydrogen per surface beryllium. Formation of similar distorted Be-H chains was also observed in the latter case. It seems that the critical coverage above which molecular adsorption stops is below the maximum hydrogen coverage, which can be reached by atomic hydrogen adsorption or diffusion of hydrogen from the bulk. Moreover, probably the maximum coverage will be reached with two hydrogen atom per beryllium corresponding to the formation of complete BeH<sub>2</sub> chains. Therefore our findings are complementary to the previous results from [29].

Theoretical study of equilibrium shape of hcp crystals was performed in a number of publications [32, 24, 25, 26].

There is plenty of experimental investigations of helium bubbles growing as a result of ion or neutron irradiation at elevated temperatures in beryllium. It is commonly accepted that helium bubbles in beryllium have a form of prism with hexagonal base



Figure 1: Minimum energy configurations of beryllium surfaces at monolayer (100%) hydrogen coverage. Only the two outermost layers are shown: the top (lightgray) and the layer beneath it (gray). Hydrogen atoms (purple) are shown at the surface. The top atoms are also called surface 'ridge', the layer beneath it – surface 'valley'.

laying on the basal plane of hcp lattice which height is smaller than width (see, e.g. [30]). The side faces of the prism are assumed to be rectangle  $\{01\overline{1}0\}$  facets. Klimenkov et. al. [14] have confirmed the hexagonal form of bubbles and showed that height to width ratio varies with the irradiation temperature. However, the prism was often truncated by one of the pyramidal planes instead of prismatic.

Sometimes quite different shape of bubbles was reported after hydrogen implantation at elevated temperatures. Implantation with deuterium ions at 500 and 700 K led to formation of faceted bubbles elongated along [0001] direction [31]. The study of hydrogen-implanted beryllium at temperature below 50°C and than annealed for 15 min at 500-600°C has revealed the elongated shape along [0001] direction and truncated by pyramidal planes [15].

Our model calculations predict change of the faceting shape of bubble with increase of hydrogen surface coverage of its walls. The area of the most energetically favorable without hydrogen basal surface is decreasing until it disappears, while the area of the pyramidal type II plane is dominating at high hydrogen coverage until other facets disappear finally.



Figure 2: Surface energy of beryllium surfaces as a function of hydrogen coverage. Zero coverage corresponds to the energy of beryllium surface without hydrogen atoms. Lines connecting the data points are guides to the eye.

The discrepancy between our prediction of equilibrium shape of bubbles with the mentioned above experimental studies in beryllium can have the following reasons:

- 1. Faceting under irradiation or implantation conditions is kinetic process which stages can be far from the expected equilibrium shape.
- 2. Presumably the hydrogen coverage can be different on different beryllium surfaces. Moreover, the coverage of the surfaces probably depends on hydrogen gas pressure in the bubble or hydrogen production rate in the bulk.
- 3. Temperature slightly changes the bubble morphology. For instance, bubbles with argon gas in hcp zinc after bombardment in heavy-ion accelerator at 300°C were bounded by basal, pyramidal type I and prismatic type I facets, while at lower temperature of 130°C the dominating facets were basal and prismatic type I [32].

### 5. Conclusions

The critical hydrogen coverage above which hydrogen molecular adsorption stops was found for all studied beryllium surfaces. At higher coverage hydrogen prefers to be two-fold coordinated with beryllium atoms, i.e. occupies mainly the bridge site above the middle of Be–Be bond. An increase of hydrogen concentration results in a significant reduction of surface energy for all surfaces except prismatic type II, which energy changes only moderately. At monolayer coverage a pyramidal type II plane was found to be the most energetically favorable, while the energies of other surfaces are noticeably higher. An equilibrium shape of hydrogen covered bubbles in beryllium was studied using Gibbs-Wulff construction. The bubble without hydrogen is bounded by basal, prismatic type I and pyramidal type I planes with a small fraction of prismatic type II facet. Our model predicts drastic changes of faceting



Figure 3: Calculated equilibrium shape of bubble in beryllium at 0 K as a function of hydrogen coverage (shown below). It was assumed that hydrogen concentration is the same on different beryllium surfaces.

with hydrogen coverage so that at monolayer coverage all faces are pyramidal type II planes.

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