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Can aluminium or magnesium be a surrogate for beryllium: A critical investigation of their chemistry

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HIGHLIGHTS

- Review of the chemical and physical properties of Al, Mg and Be.
- Similarity of Be and Al oxide.
- Mg is not a good replacement for Be.

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ABSTRACT

The use of beryllium is still an existing question according to the studies concerning the plasma–wall interactions which are expected to occur in ITER. Prediction of erosion and co-deposition processes for ITER is necessary for the design and the material choice of the first wall. In the current configuration, it is expected that co-deposited layers containing Be, tungsten and possibly carbon will be formed. However, the toxicity of Be limits its use in many experimental facilities around the world. Using aluminium or magnesium as Be replacements in laboratory experiments would solve this problem of toxicity and handling of Be mixed materials. A critical question which automatically arises is the relevance to use Al or Mg regarding the physical and chemical properties of both elements in comparison to the co-deposited layers expected in ITER. This work provides a review of the chemical and physical properties of Al and Mg, in the respect of comparing these properties to those of Be. Thanks to the similarity of its electronegativity to Be, Al can successfully resemble Be in terms of formation of compounds, especially the oxides and possibly the hydrides. However, due to the difference in the nature of the bonding, Mg cannot be a replacement for a possible hydride deposit formation.

1. Introduction

Erosion and co-deposition processes have to be well preestimated for the material choice and the design of ITER first walls. The current choice of ITER materials include Be at the main wall, W at the divertor entrance and dome baffles and CFC at the strike points. With respect to this, depending on the local plasma parameters, deposits containing Be and W will form [1]. These deposits may also include C depending on the choice of the divertor material [2]. Laboratory experiments which aim to experimentally simulate ITER-like edge conditions are limited in the use of Be due to its high toxicity [3,4]. Al and Mg are two alternative elements which can replace Be in such simulations in order to avoid forming and subsequently handling these toxic deposits. A natural question which automatically arises is the relevance of the physical and chemical properties of these two elements to those of Be.

This work provides a review of the chemical and physical properties of Al and Mg, in the respect of comparing these properties to those of Be. Comparison of their nuclear properties is not included in this work. Thanks to the similarity of its electronegativity to Be, Al can successfully resemble Be in terms of formation of compounds, especially the oxides and possibly the hydrides. The presence of beryllium deuteride has been confirmed in Be co-deposited layers as well as in the plasma column of the PISCES-B experiment [5]. Due to the difference in the nature of the bonding, Mg cannot be a replacement if such a possible hydride formation exists. However, Al has covalent bonding and a comparable electronegativity value. The chemical reaction between Al with W in a deuterium plasma is presented using X-ray photoelectron spectroscopy (XPS) and compared with results investigated by the same technique for

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Be [6]. A special issue which is also addressed is the replacement of Be in plasma–wall interaction studies for the first mirrors of ITER's diagnostics [3].

2. Physical and chemical properties of beryllium, aluminium and magnesium

2.1. Physical properties

The physical properties of Be, Al and Mg are presented in Table 1. The most important differences are: The melting temperature for Be is around 600 °C higher than that of Al and Mg. Mg and Be have the same structure (hcp) and Al crystallizes in a cubic structure (fcc), the lattice structure of Mg is the closest to Be. Be and Al have low vapour pressure values. The sputtering yield by 200 eV deuterium ions is different for each element and the ion range is smaller for Al and Mg than it is for Be. The atomic spectroscopic data are given in the table as well as the resonance lines of neutral atom [7]. In summary, in terms of their physical properties, neither Al nor Mg can fully resemble Be.

2.2. Chemical properties

Table 2 summarizes the chemical properties of Be, Al and Mg. Be and Al have a comparable chemistry and they both have oxides with the same structure (Wurtzite) due to their close electronegativity values. BeO and Al_2O_3 are extremely hard and have high melting points. They are non-volatile, soluble both in acids and bases. In comparison to those, MgO is ionic. $(BeH_2)_x$ and $(AlH_3)_x$ are polymeric and covalent, MgH_2 is ionic, and they all have different melting temperatures. All elements are known to form carbides and alloys with W, Mo and Rh as listed.

3. Reaction of Al with W in a deuterium plasma and comparison to Be

In our specific setup [3] it is possible to create deuterium plasma, where methane (CH_4) can be added into the plasma, as well as some W and Al impurities by means of magnetron sputtering. With this method, deposits containing these elements were formed and transferred without breaking the vacuum to an ultra-high vacuum chamber housing a photoelectron spectrometer for XPS measurements. Experiments were presented in our previous paper [3]. In Fig. 1, the Al2p and W4f core level spectra for the deposits obtained from carbon free plasma mixtures are plotted. For the films Al-1 and Al-3, the depositions were performed with Al and W magnetrons running simultaneously, whereas for the Al-2 film no W was sputtered. In order to increase the deposition rate, Ar gas was added in the deuterium plasma. Al-1, 2 and 3 were deposited with 0, 10 and 46% (partial pressure percentage) of Ar, respectively. The Al2p peak for 0% of Ar appears only at the oxide position [8]. Increasing the percentage of Ar leads to an increase of the metallic components both for Al or W. A possible alloy formation between Al and W, or with the substrate is not investigated for the time being.

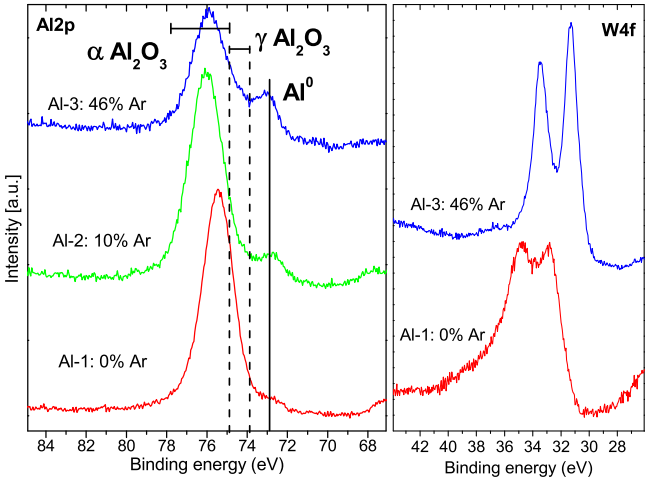

Fig. 1. Al2p and W4f core level spectra measured by in situ XPS for various deposits formed on molybdenum substrate with a variable percentage of Ar in the deuterium plasma. The shown spectra are normalized for comparison. The vertical lines are given as eye guides for the binding energy of Al metal, and the energy ranges of α and γ Al_2O_3.

The typical background pressure in our setup is around is around 5×10^{-5} Pa. The deposited films appeared as oxides due to the residual species in the chamber especially, for gas mixtures with low percentages of Ar in the plasma. We think that the electropositive Al adatoms reacted with electronegative oxygen faster than they coalesce with each other, resulting in heavily oxidized deposits [3]. A comparable effect is observed also for W4f peak for the Al-1 sample (Fig. 1).

Be also has a very high reactivity towards O-containing species, forming BeO. Therefore, surface chemistry studies with it have to be carried out under very good vacuum conditions (low 10^{-9} Pa range). Very fast oxidation rates with molecular oxygen are observed up to BeO thicknesses of 2–3 monolayers only, for H_2O the oxidation continues [9]. For atomic oxygen, the oxidation rates are even faster [10]. In contrast to Al_2O_3, BeO layers allow the diffusion of Be through the oxide layer to the surface (with possible continuing oxidation) above temperatures of 600 °C [11]. With graphite deposited on a beryllium substrate, Be_2C is formed upon annealing above 400–500 °C. Even at higher temperatures, no dissolution of C into the Be substrate is observed [12]. However, above 800 °C, Be_2C layers on Be substrates (Be_2C layers on graphite only above

Table 1
Physical properties of beryllium, aluminium and magnesium.

	Beryllium	Aluminium	Magnesium
Melting point (°C)	1287	660	650
Lattice structure	hcp	fcc	hcp
Lattice constants (Å)	$a = b = 2.28$ $c = 3.60$	$a = b = c = 4.06$	$a = b = 3.18$ $c = 5.15$
Density (g/cm^3)	1.85	2.7	1.74
I Ground state	$1s^2 2s^2\ ^1S_0$	$1s^2 2s^2 2p^6 3s^2 3p\ ^2P_{1/2}$	$1s^2 2s^2 2p^6 3s^2\ ^1S_0$
Ionization energy (eV)	9.3	6.0	7.6
II Ground state	$1s^2 2s^1 S_{1/2}$	$1s^2 2s^2 2p^6 3s^2\ ^1S_0$	$1s^2 2s^2 2p^6 3s\ ^2S_{1/2}$
Ionization energy (eV)	18.2	18.8	15.0
Spectroscopic line I Ground state and wavelength (nm)	$2s^2$–2s2p (234.8)	$3s^2 3p$–$3s^2 4s$ (396.1)	$3s^2$–3s3p (285.2)
Cohesive energies (eV)	3.3–3.7	3.4	1.5
Young's modulus (GPa)	287	70	45
Temp. for 1 Pa vapor pressure (°C)	1189	1209	428
Sputter yield by 200 eV D^+ ions (10^{-3}atoms/ion)	45	37	49
Ion range for 200 eV D^+ ions (Å)	17	9	9