4th Asia-Pacific Conference on Plasma Physics, 26-31Oct, 2020, Remote e-conference

The effect of O impurity particle adsorption on the Cs/Mo (110) surface

Heng Li[1], Xin Zhang[1], Yuhong Xu[1], Guangjiu Lei[2], Changjian Tang[1,3] Katsuyoshi Tsumori[4], Shoichi Okamura[4], Mitsutaka Isobe[4], Akihiro Shimizu[4], Qijun Liu[5], Yuxiang Ni[5], Zilin Cui[1], Yangyang Liu[1], Ming Li[2], Shaofei Geng[2], Haifeng Liu[1], Xianqu Wang[1], Jie Huang[1], Hai Liu[1], Jun Cheng[1] and CFQS team[1,4]

[1]Institute of Fusion Science, School of Physical Science and Technology, Southwest Jiaotong University, Chengdu, 610041, People's Republic of China.

[2]Southwestern Institute of Physics, Chengdu, 610041, People's Republic of China.

[3]School of Physical Science and Technology, Sichuan university, Chengdu, 610041, People's Republic of China.

[4]National Institute for Fusion Science, National Institutes of Natural, Science, Toki, 5095259, Japan.

[5]School of Physical Science and Technology, Southwest Jiao tong University, Chengdu, 610031, People's Republic of China.

e-mail: hengli@my.swjtu.edu.cn

Abstract

Neutral beam injection (NBI), which is one of the means to heat the plasma and drive the plasma current, is an important facility in tokamaks and stellarators. NBI can be divided into N-NBI and P-NBI due to the difference in charge property of the accelerated particle, and the N-NBI is regarded as the most efficient one. In a large source of N-NBI, surface production of negative ions is considered to be the most efficient way. The lower the work function of the surface, the higher the efficiency of negative ion generation [1]. The coverage of Cs atoms can significantly reduce the work function of metal surfaces. When Cs coverage is 0.6 monolayer, the work function of Mo metal surface will reach the minimum value [2]. Generally, in addition to cesium, there would are some other impurity particles, such as O, W, and C [3]. How these impurity particles affect surface properties that need to be understood through computational or experimental data.

In this work, the O impurity particle adsorption on the Cs/Mo(110) surface, to determine the influence of O on Cs stability on Mo(110) surface and also the work function of Cs/O/Mo(110) surface, has been investigated by performing density functional theory (DFT) [4]. There are four independent adsorption sites on Cs/Mo(110) surface for O atom. No matter which adsorption site O was adsorbed, the surface adsorption energy of Cs increased. O atoms attract more charges due to the difference in electronegativity. Although this weakens the interaction between the Cs and Mo atoms, the O atom does connect them like a bridge, resulting in enhanced adsorption of Cs atom. In our model, the surface work function of Cs/Mo(110) is calculated as 1.835 eV. In some cases, the adsorption of O can dramatically reduce the surface work function to 1.633 eV. Conversely, O may also increase it, but this increase is not pronounced. This result suggests that the appropriate addition of O atoms may be beneficial to the development of high-efficiency negative ion sources.

References

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