Accepted Manuscript

Ab initio molecular dynamics simulation of the effect of impurities on laser-induced damage of fused silica

Qingyi Feng, Li Li, Tuqiang Zeng, Mingwen Zhang, Jinlan Nie, Haiyan Xiao, Rui Su, Xiaotao Zu

PII: S0921-4526(18)30363-6

DOI: 10.1016/j.physb.2018.05.029

Reference: PHYSB 310891

To appear in: *Physica B: Physics of Condensed Matter*

Received Date: 16 April 2018

Revised Date: 20 May 2018

Accepted Date: 21 May 2018

Please cite this article as: Q. Feng, L. Li, T. Zeng, M. Zhang, J. Nie, H. Xiao, R. Su, X. Zu, Ab initio molecular dynamics simulation of the effect of impurities on laser-induced damage of fused silica, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.05.029.

Ab initio molecular dynamics simulation of the effect of impurities on laser-induced damage of fused silica

Qingyi Feng[12], Li Li[1*], Tuqiang Zeng[1], Mingwen Zhang[1], Jinlan Nie[1], Haiyan Xiao[1], Rui Su[2], Xiaotao Zu[1]

1 School of Physical Electronics, University of Electronic Science and Technology, Chengdu 610054, China

2 Research Center of Laser Fusion, China Academy of Engineering Physics, Mianyang 621900, China

Abstract: The damages of fused silica surface after laser irradiation can be caused by the impurities introduced during manufacture processes. In this paper, Fe and Ce impurities are considered in fused silica. The first-principles method is employed to simulate the process of high-power ultraviolet laser irradiation to fused silica. The bond angle distribution, pair distribution function, the density of state (DOS) and other information of fused silica structures are calculated. There is a remarkable difference in bond length and bond angle distribution between pure and doped fused silica. New defect states are also observed in DOS with the narrower band gap, and new optical absorption peaks appear in the dielectric function for the fused silica with the dopants after laser irradiation. This means that fused silica with impurities has more significant absorption for laser energy than pure fused silica. Fe-O bonds are found more stable than Ce-O ones after irradiation. This indicates the damage of Fe doping is greater than that of Ce doping. So, doping of metal indeed leads to a decrease in damage resistance to laser for fused silica, and Fe is more harmful than Ce.

Keywords: fused silica; first-principle; irradiation; impurity; laser-induced damage

1. Introduction

Fused silica is usually used as the optical components in the ignition devices of Inertial Confinement Fusion (ICF) [1]. With the high-power ultraviolet (UV) laser irradiation, fused silica lens are extremely prone to fracturing, melting, carbonating and other macro-damages which can reduce the resistance to laser. And this is a significant negative impacts to the stable operation of the

* Corresponding author. Tel: +86 028 83202130.
E-mail address: jasmine2008@uestc.edu.cn.