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Ab initio molecular dynamics simulation of the effect of impurities on

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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

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