Density Functional Theory Study of Gas Adsorption on Lanthanum Zirconate Nanostructured Coating Surface

Xingye Guo[1], Jing Zhang[1], Yeon-Gil Jung[2], Li Li[3], James Knapp[3]

[1] Department of Mechanical Engineering, Purdue School of Engineering and Technology, Indiana University-Purdue University Indianapolis

[2]School of Materials Science & Engineering, Changwon National University, Changwon, Gyeongnam 641-773, South Korea

[3]Praxair Surface Technologies Inc., Indianapolis, IN 46222, USA

Lanthanum zirconate ($La_2Zr_2O_7$) is a typical pyrochlore ceramic material, which can be used as thermal barrier coating (TBC). However, it may deteriorate by oxidizing and corrosive gases, such as CO_2, O_2, SO_2 and CH_4 during its operation process at elevated temperatures. This work investigates CO_2, O_2, SO_2 and CH_4 gas adsorption mechanism on $La_2Zr_2O_7$ nanostructured coating surfaces using the density functional theory (DFT) calculations. $La_2Zr_2O_7$ surface energies on (001), (011) and (111) planes were calculated. Results show the most thermodynamically stable surfaces of $La_2Zr_2O_7$ are (011) and (111) planes, due to their low surface energies. Adsorption energies of CO_2, O_2, SO_2 and CH_4 on (001), (011) and (111) planes in different sites were studied as well. The results show the most favorable gas adsorption sites for CO_2, O_2, SO_2 and CH_4 occur at 3-fold and 4-fold sites. The most favorable gas adsorption plane for CO_2, O_2, SO_2 and CH_4 is (111) plane.