# STUDY OF THE THERMAL AND MECHANICAL PROPERTIES OF $LA_2ZR_2O_7$ USING FIRST PRINCIPLE METHOD

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As an advanced thermal barrier coating, Lanthanum zirconia ($La_2Zr_2O_7$) has been studied in this paper using first principle calculations. $La_2Zr_2O_7$ crystal bulk was used in this calculation. The lattice parameter, mechanical and thermal properies of $La_2Zr_2O_7$ were investigated by means of density functional theory (DFT). Hydrostatic pressure-dependent elasticity constant, bulk modulus were calculated. The thermal conductivity was calculated based on fick's law using a 20 layers supercell. $La_2Zr_2O_7$ coating samples were spraied by APS equipment, the coating samples were identified by XRD and observed by optical microscope. The thermal effect of Ce doping of the $La_2Zr_2O_7$ were studied by ab initial calculations. The calculated properties have considerable good agreement with others experimental and calculation results.