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# The compression behaviors of zirconium from the first - principle calculations

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**Abstract.** Investigation into the structural, elastic and electronic properties for pure zirconium(Zr) crystal had been conducted by the first-principles pseudopotential method based on density functional theory. Both methods, local density approximation (LDA) and generalized gradient approximation (GGA), had been applied on the geometrical optimization of pure Zr to address the difference between two methods and their applicabilities. The result elucidated LDA could match the experimental data better, compared with method GGA. What's more, the structural properties under pressure had been stimulated and analyzed, showing crystal lattice parameters and crystalline volume change nonlinearly within the external pressure. In contrast, the single point energy of Zr showed a great linear correlation with the changing pressure. The elastic constants of the pure Zr were calculated, proving that Zr would acquire excellent ductibility and mechanical stability under pressure. In addition, the optical properties of zirconium under different pressures were analyzed. The adsorbing coefficient increased with the increasing pressure.

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**Key words**: zirconium, first principles, mechanic properties, optical properties

## 1 Introduction

The key components of the space craft were mostly made by high hardness steel and sometimes dopped with titanium alloy. However, near over 40 spacial exposure experiments showed us these traditional materials have no means to meet the need for the

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space craft in rigorous space condition, which caused people to find more light kind of materials, and metal Zr and its alloy might be thought as more suitable for aerospace materials, since it enjoys uncompetitive aerospace applicability . First, zirconium's excellent resistance to corrosion and low neutron-capture cross-section make it suitable for working in the space with extremely severe corrosion such as energetic particle radiation [1]. The melting spot of titanium alloy is about 1600 °C, however, it is higher than 1800 °C for zirconium alloy. Thanks to its great heat resistant ability, Zr and its oxide have been popular applied in the production and design of aerospace craft [2–4]. Second, to achieve the real space application of the moving parts from the space crafts, the key is to achieve the strengthening-toughening and lightweight of the space materials. The strength of zirconium alloy when dopped with a small amount of Sn and Nb, can reach over 900 MPa. Besides, the ductility of pure zirconium is extremely high with extensibility as 35%. So the zirconium alloys system had thus powerful strengthening-toughening potential applications. Simultaneously, the density of pure zirconium is lower than steel by 16%, it can be easily alloyed with some light metals. Many theoretical works had been conducted for pure Zr and Zr-based alloys. Jakse *et al.* investigated the local structure and its change during its undercooling by means of the first principle molecular dynamics simulations. Furthermore, the research shows that for Zr, an increasing degree of a body center cubic (bcc) type ordering upon undercooling occurs, in relation to the structure of the high temperature solid phase [5]. Hui *et al*. studied that the energies, pair correlation functions, structural factors and distribution of bond pairs during the liquid-solid transition of Al and Zr by ab-initio molecular dynamics simulation. Liquid Zr transforms to thermodynamic stable bcc phase and glassy structure around 1200 K, when cooled at average rate of $4.3\times10^{13}$ and $2.0\times10^{14}$ K/s respectively. And it is also shown that the structures of liquid and glassy Zr are mainly composed of icosahedral and bcc type of short range orders [6]. The composition dependence of the structural and dynamical properties of Zr-Ni alloys had also been studied by molecular dynamics simulations [7]. What's more, our group also focused on the study of zirconium binary alloy, especially the structural properties of $Zr_2Al$ under pressure [8]. Kawamoto *et al*. [9] investigated the scaling trends of band offsets at model Zr-Si interfaces, and found that the band gap and band offset decreased as the concentration of Zr increased. As for ternary alloys, the glassy forming stability of $Cu_{46}Zr_{46}A_{l8}$ and $Fe_{78}M_9B_{13}$ (M=Nb, Si, Zr) were investigated with ab-intio method [10,11]. The former one is mainly based on correlation function, Warren-Cowley parameters, as well as topology short program, to describe its glassy structure. Zr-based alloys had been investigated deeply by experimental and theoretical method. In contrast, the latter one compared the structural and dynamical properties of $Fe_{78}Nb_9B_{13}$ $Fe_{78}Z_9B_{13}$ and how the properties influence their glass forming ability, mainly based on the melting structure of $Fe_{78}Si_9B_{13}$. However, to the best of our knowledge, so far, few experimental or theoretical results had been reported for pure Zr metal. Under such motivation, we attempt to give a detailed theoretical study on structural, elastic, electronic and thermal properties by using first-principles plane-wave method.

In this paper, we firstly investigated Zr within 0-50 GPa using two exchange corre-