Journal of Nuclear Materials 458 (2015) 122–128

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Ab initio calculations of the ideal tensile and shear strengths of uranium metal

Jin-Wen Yang [a,b], Tao Gao [a,c,*], Ben-Qiong Liu [d], Guang-Ai Sun [d], Bo Chen [d]

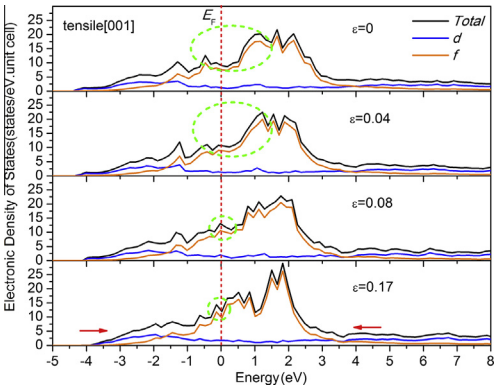
[a] Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China
[b] Department of Physics, Taiyuan Normal University, Taiyuan 030031, China
[c] Key Laboratory of High Energy Density Physics and Technology of Ministry of Education, Sichuan University, Chengdu 610064, China
[d] Key Laboratory of Neutron Physics, Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621900, China

HIGHLIGHTS

- The ideal tensile strengths have been investigated.
- The ideal shear strengths have been investigated.
- Tensile and shear processes are associated with the transformation of electronic structure.
- *Cmcm* uranium exhibits a high degree of mechanical anisotropy.

GRAPHICAL ABSTRACT

The total and partial DOS as a function of tensile strains along the [001] direction.



ARTICLE INFO

Article history:
Received 10 September 2014
Accepted 9 December 2014
Available online 17 December 2014

ABSTRACT

The mechanical properties under large tensile and shear strains for orthorhombic uranium have been investigated systematically using the *ab* initio Density Functional Theory (DFT). We calculated the ideal tensile and shear strengths by incrementally deforming the simulation cell using first-principles total energy method. The obtained ideal tensile strengths are 21.3, 14.9, and 12.8 GPa in the [100], [010], and [001] crystalline directions, respectively, and the obtained ideal shear strengths are 14.3, 7.8, and 8.9 GPa in the (100)[011], (010)[101], and (001)[110] slip systems, respectively. In both cases, the present calculated results present typical mechanical anisotropy in different orthorhombic axes and slip systems. In particularly, the calculated electronic density of states (DOS) and the charge density of *Cmcm* uranium under the loading conditions consistently demonstrate that both tensile and shear deformation processes are intrinsically correlated with the evolution of electronic structure.

1. Introduction

Uranium has attracted considerable interest over many years, the main reason is its growing importance as an essential component of nuclear weapons and reactor fuel [1–5]. Uranium is an electron-correlation metal with a partially filled 5*f*-electron

* Corresponding author at: Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China. Tel./fax: +86 28 85405234.
E-mail address: gaotao@scu.edu.cn (T. Gao).

http://dx.doi.org/10.1016/j.jnucmat.2014.12.037
0022-3115/

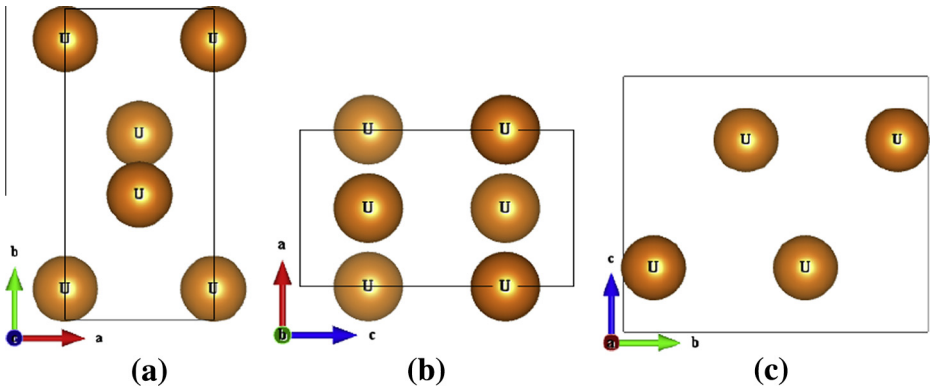


Fig. 1. The orthorhombic *Cmcm* structure of uranium in a unit-cell. (a) The atom projection in the *ab* plane; (b) the atom projection in the *ac* plane; (c) the atom projection in the *bc* plane.

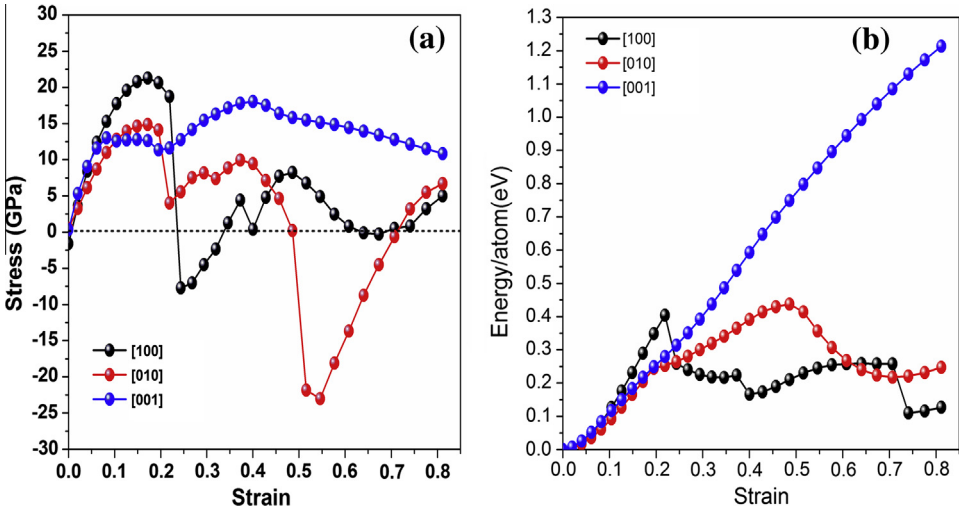


Fig. 2. Stress–strain (a) and energy-strain (b) curves of α—U for the [100], [010], and [001] uniaxial tension.

Table 1
Calculated ideal tensile strength σ_m (in GPa) and corresponding strain ε_m (%), as well as V/V_0 in the three different directions of α—U.

Directions	Present calculations		
	σ_m	ε_m	V/V_0
[100]	21.3	17.2	1.12
[010]	14.9	17.2	1.08
[001]	12.8	14.9	1.05

shell, this crystal presents rich phases. Especially, the anomalous physical characteristics of the alpha-phase have made it a subject of much interest for scientific research. The structure of α—U is remarkably stable, there is no phase transition up to 100 GPa in a diamond-anvil cell (DAC) measurement [6]. Its elastic constants at room temperature have been obtained from experiment reported by Fisher and McSkimin [7] and calculations from First-principles simulations at zero temperature using different methods by some groups [3,5,8,9].

α—U belongs to No. 63 space group with the orthorhombic *Cmcm* structure, it is very essential to determine its mechanical anisotropy. The knowledge of the tensile and shear anisotropy, even the anisotropy of directional bulk modulus and Young's modulus could provide much valuable information for exposing the nature of mechanical properties, such as load deflection, fracture toughness, and even thermoelastic stress. The ideal or theoretical strength of materials is the stress which is required to force deformation or fracture at the mechanical instability [10], that is to say, the ideal strength is that a perfect single crystal free of any defects becomes unstable with respect to fracture by the spontaneous separation of atomic planes, this physical quantity sets an upper bound on the attainable stress of crystals [10]. Both high strength and good ductility are the most crucial characteristics of metallic materials. Ordinarily, mobile dislocations, grain boundaries, shrinkage cracks, and other microstructural features may control the ideal strength of a real material, but they can never raise it above its ideal value [10]. At present, *ab* initio density-functional calculations method has been successfully performed to compute the ideal strengths of many materials, including FCC Al, Cu, Ag, Ni metals, BCC W, Mo, and Fe metals, HCP Mg, Ti, and Zn metals [11–13], diamond cubic C, Si, Ge, and *c*—BN [14,15], β—SiC, α—Si_3N_4, β—Si_3N_4, B1—NaCl, MgO, KBr, CaO compounds [13], and even some grain boundaries [16,17], etc.

Up to now, the tensile and shear properties of α—U have not been investigated, its mechanical properties under deformation are poorly known, there is still a lack of a systematic understanding for the stress–strain relations of α—U, so it is necessary to investigate its deformation process related with the mechanical failure modes under tensile and shear strains. Hence, we adopt Density Functional Theory (DFT) to study the mechanical behavior of orthorhombic α—U under large tensile and shear strains, then to