AB INITIO MODELLING DEFORMATION OF PERFECT CUBIC CRYSTALS UNDER TRIAXIAL TENSION

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ABSTRACT

Ab initio calculations of ideal strength of cubic crystals under three-axial tension are performed using the LMTO-ASA method. Two exchange-correlation term approximations (LDA, GGA) were applied. Computed values are compared with those obtained previously by means of semi-empirical approach. Values of equilibrium lattice parameter obtained in the framework of ab-initio method are well comparable with experimental data whereas a less satisfactory agreement was achieved in case of bulk moduli and cohesive energy.

KEYWORDS

Ideal strength, ab initio calculations, LMTO-ASA.

INTRODUCTION

Ideal (or theoretical) strength (IS) values represent upper strength limits for a given solid under a given loading type. The three-axial (hydrostatic) tension value σ_{id} is very useful for the crack stability assessment in solid crystals (SC) since the three-axial tension stress state exists at the crack tip. On the other hand, experimental verification of σ_{id} values is extremely difficult and, as far as we know, no plausible data are available till now.

The aim of this article is to use a selected ab initio approach for calculation of σ_{id} values of cubic crystals and to compare them with results obtained by semiempirical methods. Values of equilibrium lattice parameter a_0 and bulk modulus K are also calculated by means of this approach and compared with experimental data. This assesment is useful for examining reliability of the particular computational method.

COMPUTATIONAL DETAILS

In this work, the Linear Muffin-tin Orbitals (LMTO) method is used in the framework of an Atomic Sphere Approximation (ASA) [1]. This method is particularly suitable for closely packed structures like f.c.c. or b.c.c. [2] and a loading type keeping the unchanged symmetry. The exchange-correlation contribution is evaluated in frame of both Local Density Approximation (LDA) and Generalised Gradient Approximation (GGA). The scalar-relativistic approach was used to include relativistic effects (particularly for heavier elements). Number of k-points in the whole Brillouine zone has been set to 4096, s, p, d orbitals were included into hamiltonian matrix and f orbitals were downfolded [3].

Behaviour of crystals in our calculations is characterized by the dependence of the total energy E_{tot} per atom on the normalized volume ν. This function was constructed by

means of a cubic spline interpolation based on a number of E_{tot} values corresponding to different values of lattice parameter a for each cubic crystal.

As it has been shown in [4, 5], IS can be evaluated using relation

$$\sigma_{id} = \frac{n}{a_0^3} \frac{\mathrm{d}E_{tot}}{\mathrm{d}\nu}\bigg|_{\nu=\nu_{pi}} .$$

Here n is the number of atoms in the elementary cell, $\nu = a^3/a_0^3$ is the normalized crystal volume, a is the lattice parameter and a_0 is its value in the unstressed state ($\sigma = 0$).

The bulk modulus K can be obtained according to the formula

$$K = \frac{n}{a_0^3} \frac{\mathrm{d}^2 E_{t1}}{\mathrm{d}\nu^2}\bigg|_{\nu=1} .$$

The cohesive energy U is calculated as a difference between energy of a free atom and that of the atom in a crystal environment.

RESULTS AND DISCUSSION

Values σ_{id} for all investigated crystals are listed in Table 1. For comparison, values obtained from semi-empirical approaches based on some empirical potential approximations are also listed for all investigated crystals. The correlation between results achieved by means of the LMTO-ASA and the polynomial approach (originally introduced in [6]) is shown in Fig. 1.

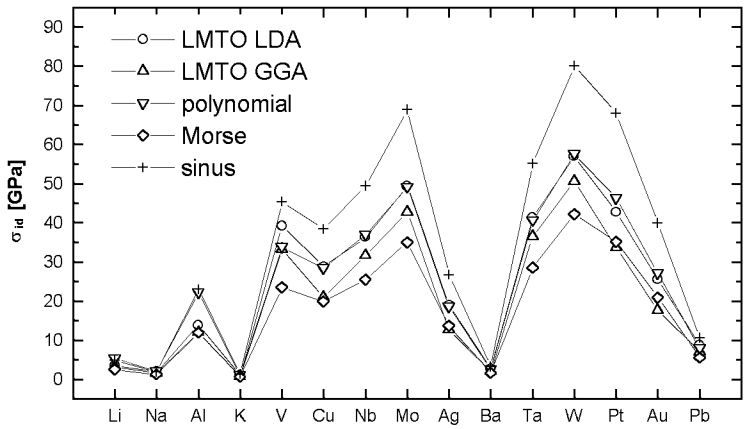

Figure 1: IS values in various approximations

It can be seen from Table 1 and Fig. 1 that the σ_{id} values obtained by means of LMTO LDA and polynomial approaches are mostly in good agreement. This conclusion is supported also by recent results [7] achieved using the Discrete Variation Cluster Method (DVM) also listed in Table 1. The simple sinusoidal approximation leads mostly to higher σ_{id} values and the Morse approximation to systematically lower ones. On the other hand, GGA gives lower values than LDA comparable similarly with polynomial and Morse approximation. To examine reliability of the results, we should compare some other calculated properties of crystals with experimental data.

Table 1: Ideal strength in various approximations

element		Ideal strength σ_{id} [GPa]					
		LMTO		semiempirical methods			DVC
		LDA	GGA	polynomial	Morse	sinus	
Li	bcc	3.53	3.13	5.29	2.49	4.91	1.92
Na	bcc	1.97	1.55	1.96	1.20	1.86	1.77
Al	fcc	13.8	12.0	22.1	11.9	23.0	
K	bcc	0.955	0.701	1.03	0.659	1.28	0.10
V	bcc	39.2	33.2	33.8	23.5	45.4	38.3
Cu	fcc	28.8	20.9	28.4	19.9	38.4	
Nb	bcc	36.3	31.6	36.9	25.5	49.4	34.1
Mo	bcc	49.3	42.7	49.1	35.0	68.9	42.2
Ag	fcc	19.0	12.6	18.6	13.7	26.7	
Ba	bcc	2.69	1.93	2.46	1.64	3.17	
Ta	bcc	41.3	36.4	40.6	28.5	55.1	41.3
W	bcc	57.0	50.6	57.5	42.2	80.1	53.1
Pt	fcc	42.7	33.6	46.3	35.1	68.0	
Au	fcc	25.5	17.6	27.1	20.9	39.9	
Pb	fcc	8.70	6.98	7.91	5.47	10.6	

Computed values of the equilibrium lattice parameter a_0 are shown in Table 2 together with experimental data [8]. The ratio a_{ip}/a_0 expresses the lattice deformation corresponding to the point of inflection of the $E_{tot}(\nu)$ curve, i.e. gives the strain at the moment of achieving the ideal strength of a relevant SC. (Only LDA values are present here, but there is a very small diference between LDA and GGA results).

Lattice parameters corresponding to the minimum of the E_{tot} vs. ν curves lie within a range of 2% when compared LDA results with experimental data [8, 9] with the exception of alkali metals where the difference represents 4% to 6% and Ba (8%). The relative elongation of the lattice parameter for SCs at the point of inflexion is usualy about 15%. As can be seen from Table 2, better agreement is achieved in case of GGA calculations, because the maximal difference between calculations and experiment is only 3%.

Computed and experimental values of bulk modulus K are listed in Table 3, where values obtained by other two ab initio calculations taken from [7] and [10] are also included.

Table 2: Lattice parameters in minimum of $E_{tot}(v)$

element	lattice parameter a_0 [Å]			a_{ip}/a_0
	LMTO LDA	LMTO GGA	Experiment	(LDA)
Li	3.34	3.49	3.50	1.22
Na	4.02	4.20	4.29	1.20
Al	3.97	4.04	4.05	1.15
K	5.00	5.30	5.23	1.19
V	2.94	3.01	3.03	1.17
Cu	3.51	3.63	3.61	1.14
Nb	3.26	3.33	3.30	1.17
Mo	3.13	3.18	3.14	1.15
Ag	3.99	4.13	4.08	1.12
Ba	4.63	5.02	5.02	1.24
Ta	3.27	3.34	3.30	1.17
W	3.15	3.21	3.16	1.16
Pt	3.90	3.98	3.91	1.13
Au	4.04	4.17	4.04	1.11
Pb	4.89	5.04	4.95	1.11

Experimental values were obtained by means of the generalized relation

$$K = \frac{1}{3}(c_{11} + 2c_{12} - \sigma)$$

in case of $\sigma = 0$ [11]. Values of elastic constants c_{11} and c_{12} were taken over from [8, 9, 12]. Computed values of the bulk modulus K lie mostly within the range of 15% in comparison with those obtained experimentally. It should be mentioned, however, that even experimental values for ambient temperature taken from different sources exhibit a scatter within the range of about ±5%. Additional deviations would appear due to the extrapolation down to the zero temperature particularly in case of alkali metals.

Values of cohesive energy are listed in Table 4. It is evident, that LMTO LDA results are systematicaly higher than experimental values. Use of GGA leads to lower values and improves the agreement with experiment. Then the differencies are mostly smaller than 20%.

In general the GGA in the framework of the LMTO-ASA method yields results reason-

Table 3: The values of bulk modulus K

element	K [GPa]					
	LMTO LDA	LMTO GGA	DVC	KKR	Experiment	
Li	16.0	15.0	10.6	15.0	13.3	[78 K]
Na	9.90	7.40	6.96	9.0	7.70	[50 K]
Al	88.8	76.1			88.2	[0 K]
K	4.90	3.84	3.07	4.0	3.70	[50 K]
V	211	185	205	164	162	[0 K]
Cu	202	146		155	145	[0 K]
Nb	185	172	166	168	170	[293 K]
Mo	272	289	263	251	270	[77 K]
Ag	149	103			109	[0 K]
Ba	7.34	10.8			10.3	[293 K]
Ta	216	202	188		194	[293 K]
W	304	295	286		313	[77 K]
Pt	330	250			278	[293 K]
Au	202	156			180	[0 K]
Pb	54.6	47.4			43.0	[0 K]

ably comparable with experiment. Therefore, calculated values of σ_{id} according to this approximation can be considered to be most plausible.

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Table 4: Values of cohesive energy U

element	Cohesive energy U [eV/atom]		
	LMTO LDA	LMTO GGA	Experiment
Li	2.15	1.82	1.63
Na	1.54	1.20	1.11
Al	4.38	3.31	3.39
K	1.25	0.932	0.934
V	9.64	7.90	5.31
Cu	4.93	3.57	3.49
Nb	11.5	9.57	7.57
Mo	12.3	10.20	6.82
Ag	3.95	2.60	2.95
Ba	2.48	1.67	1.90
Ta	11.0	9.01	8.10
W	12.8	10.5	8.90
Pt	7.69	5.58	5.84
Au	4.61	2.98	3.81
Pb	4.28	3.22	2.03

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