

MECHANICAL STABILITY AND ELASTIC PROPERTIES OF SOME FCC METALS: A MANY- BODY POTENTIAL APPLICATIONS

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Abstract- To represent the total energy of fcc metals (Cu, Ag, Al, Ca, Sr) the potential functions are assumed to be composed of the two-body pairwise Rydberg potential and volume dependent energy (P_1V) which represent many body interactions. Energy, stress and elastic moduli calculations are performed on the basis of Rydberg and Rydberg plus P_1V potentials to locate the stress-free bcc phase on the fcc metals. The studied crystals are subjected to unconstrained (100) uniaxial tension and compression for all computations. Also, these potentials are used to calculate the second- and third-order elastic constants, C_{ij} and C_{ijk} . The obtained results are compared with the available experimental data and the agreement is good.

Keywords: Theoretical strength, mechanical stability, many-body potential, elastic constants

1. INTRODUCTION

The studies of elastic instability of crystals were motivated by many interesting problems, such as, structure phase transformation, the prediction for liquid melting point, theoretical strength and the test for any constructed interatomic potential function [1]. Computer simulation techniques are powerful tools which have been used for many years to study the structure and properties of materials. The basic input to these simulation techniques, whether they are static methods or dynamic calculations, such as Monte Carlo and molecular dynamics, is knowledge about the interatomic potential function among particles in the system under investigation. These potentials which are used to simulate a particular material should be capable of reproducing some of the basic properties of the material. Among the material properties there are structure and lattice constants.

Born and many other investigators [1-13] noted the importance of examining the stability of crystals and have performed some theoretical strength calculations. The calculation method used in this study is a generalized form of that derived for pairwise potentials by Milstein [2]. The pairwise potential model is not adequate, so in this study, the two-body pairwise Rydberg potential [14] and volume dependent energy $\sum_n P_n V^n$

are assumed to represent the total energy of fcc crystals as in R. Najafabadi and G. Kalonji [7].

In this work by using this potential functions some theoretical calculations are performed. The stability and phase transitions, the variation of energy, stresses and elastic moduli with respect to the lattice parameters are studied. By the means of the obtained curves, the lattice parameter, atomic volumes, cohesive energies in the fcc and bcc phase and the difference of energies ($E_{fcc} - E_{bcc}$) are computed and regions of stability are determined. By using this method, some elastic properties, such as, the second-, and third-order elastic constants (C_{ij}, C_{ijk}) are also calculated.

2. COMPUTATIONAL PROCEDURE AND APPLICATIONS

2.1 Potential Function

Total interaction energy used in this work is assumed to be in the form of

$$\phi(r) = -D[1 + b(r - r_o)]e^{-b(r-r_o)} + \sum_n P_n V^n \quad (1)$$

where D , b and r_o are the potential parameters in the Rydberg potential. These are calculated by Varshni Y.A.[14] following the procedure given by Girifalco and Weizer[15]. For the volume dependent energy term, $(\sum_n P_n V^n)$ which represent many

body interactions, we choose $n=1$, and P_1 is a coefficient which depends upon the material and is calculated such that the lattice constants at zero stress match the ones observed experimentally [7]. The calculated results for D , b , r_o [14] and our results for P_1 for Cu, Ag, Al, Ca and Sr are listed in Table 1.

2.2 Mechanical Stability

For the crystals to be in stable equilibrium, the total energy of system in the presence of the applied forces must be at its minimum.

The difference in the internal potential energy between the states a_i' and a_i can be expressed in terms of a Taylor series expansion as

$$U(a_i') = U(a_i) + \sum_{i=1}^6 \frac{\partial U}{\partial a_i} \bigg|_{a_i} (a_i' - a_i) + \frac{1}{2} \sum_{i=1}^6 \sum_{j=1}^6 \frac{\partial^2 U}{\partial a_i \partial a_j} \bigg|_{a_i} (a_i' - a_i)(a_j' - a_j). \quad (2)$$

The deformations $a_i' - a_i$ are taken to be small, so that the series is truncated at second-order terms. For convenience, let

$$B_{ij} = \frac{\partial^2 U}{\partial a_i \partial a_j} \bigg|_{a_i} \quad (3)$$

and

$$F_i = \frac{\partial U}{\partial a_i} \bigg|_{a_i} \quad (4)$$

The double sum in equation (2) will be positive for an arbitrary deformation $a_i' - a_i$. This is performed only if the principal minors of determinant $|B_{ij}|$ are all positive [16]. The principal minors of the matrix B can be positive if the following conditions at state a_i are satisfied

$$\begin{aligned} B_a &= B_{22}^2 - B_{23}^2 > 0 \\ B_b &= B_{11}(B_{22} + B_{23}) - 2B_{12}^2 > 0 \\ B_{55} &> 0, \quad B_{44} > 0, \quad B_{22} > 0, \quad B_{23} > 0 \end{aligned} \quad (5)$$

In order to calculate the response of the unit cell to a uniformly applied stress along the edge a_1 , one increase or decrease the lattice constant along edge a_1 by small amount

$\Delta a_1 (\frac{\Delta a_1}{a_1} \ll 1)$ starting from the zero stress condition ($F_1=F_2=F_3=0$). The required force

F_1' to keep the unit cell at mechanical equilibrium as well as the change in lattice constant along a_2 and a_3 are calculated from equation (4). The uniform stress (σ_1) is calculated by using the following equation

$$\sigma_1 = \frac{F_1'}{(a_2')^2} \quad (6)$$

These values are defined in equations (3) and (4) in terms of derivatives of the potential function U , where U is made up of two terms U^p and U^d . The potential energy due to pair interaction per unit cell is

$$U^p = \frac{1}{2} n \sum_j \phi(r_j) \quad (7)$$

where n is the number of atoms per unit cell and r_j is the distance from an arbitrary atom in the crystal which is chosen as the origin, to the j th atom. This distance in a fcc crystal which is subject to uniform deformations may be written as

$$r = \frac{1}{2} (a_1^2 l_1^2 + a_2^2 l_2^2 + a_3^2 l_3^2)^{(1/2)} \quad (8)$$

where a_i is the cell length and all the l_i are integers such that $l_1 + l_2 + l_3$ must be even. The quantities F_i and B_{ij} due to the pair potential are given as

$$F_i^p = \frac{1}{4} n a_i \sum_{l_1} \sum_{l_2} \sum_{l_3} l_i^2 \frac{\partial \phi}{\partial (r^2)} \quad i = 1, 2, 3 \quad (9)$$

$$B_{ii}^p = \frac{1}{8} n a_i^2 \sum_{l_1} \sum_{l_2} \sum_{l_3} l_i^4 \frac{\partial^2 \phi}{\partial (r^2)^2} + \frac{1}{4} n \sum_{l_1} \sum_{l_2} \sum_{l_3} l_1^2 \frac{\partial \phi}{\partial (r^2)} \quad i = 1, 2, \dots, 6 \quad (10)$$

$$B_{ij}^p = \frac{1}{8} n a_i a_j \sum_{l_1} \sum_{l_2} \sum_{l_3} l_i^2 l_j^2 \frac{\partial^2 \phi}{\partial (r^2)^2} \quad i \neq j = 1, 2, 3 \quad (11)$$

The quantities F_i and B_{ij} due to the density dependent part of the potential are given as [7]

$$F_i^d = \sum_{n=0}^{\infty} \frac{n P_n V^n}{a_i} \quad i = 1, 2, 3 \quad (12)$$

$$B_{ii}^d = \sum_{n=0}^{\infty} n(n-1) \frac{P_n V^n}{a_i^2} \quad i = 1, 2, 3 \quad (13)$$

$$B_{ii}^d = \sum_{n=0}^{\infty} n P_n V^n \quad i = 4, 5, 6 \quad (14)$$

$$B_{ij}^d = \sum_{n=0}^{\infty} \frac{n^2 P_n V^n}{a_i a_j} \quad i \neq j = 1, 2, 3 \quad (15)$$

In this work, the density dependent part of potential is taken as

$$U^d = P_1 V \quad (16)$$

In this case the constant factor P_1 is calculated such that the lattice constant at zero stress matches that observed experimentally.

2.3. Elastic Constants

Second- and third-order elastic constants (SOEC and TOEC) at atmospheric pressure and 0K are evaluated adopting the general expressions given by Born[3]. At

T=0K, the calculated values of these constants are given in Table 4 and Table 5, respectively.

3. RESULTS AND DISCUSSION

On the structural phase transformation and elastic instability, the numerical calculations are performed using Rydberg potential and Rydberg potential plus volume dependent energy for Cu, Al, Ca, Ag and Sr under [100] uniaxial loading. Two- and third-order elastic constants are also included in the computations. The most of the numerical results obtained from this work are summarized in Fig1, 2, 3 and Table 2, 3, 4, 5.

Table-1 Calculated potential parameter [14] and our calculated P_I constants

Metals	$b\ (10^8\text{ cm}^{-1})$	$r_o(10^{-8}\text{ cm})$	$D(10^{-14}\text{ erg})$	$-P_I(10^9\text{ dyn/cm}^2)$
Cu	1.9962	2.8170	61.78	1.4952
Al	1.7133	3.1940	49.07	1.2067
Ag	1.9646	3.0881	57.76	1.5712
Ca	1.0791	4.9300	29.71	3.0950
Sr	1.0902	4.8799	57.76	1.5655

Energy versus lattice parameters curves are plotted in Fig.1 for Cu and Sr. In each curve there are two special points marked with circle and square, represent the minimum of energy, and the energy at inflection point through which the second-order derivative of energy with respect to a_I changes sign, respectively. Our numerical results show that the points marked with circle assert the initial equilibrium state of the fcc structure and the points marked with triangles occupies the stress- free face centered tetragonal (fct) structures. The squares indicate the stress-free bcc face phases, where the ratio a_2 to a_1 (with $a_2=a_3$) is taken to be $\sqrt{2}$.

The stress σ_I versus cell length a_I are shown in Fig.2 for Cu and Sr. The square and circle marks on the curve are associated with the stress-free cell length a_{bcc} and a_{fcc} . The values of a_{bcc} and a_{fcc} are calculated from the values of marked points, respectively. It can be seen from Table 2 that theoretical lattice parameter a_{fcc} and energy E_{fcc} of fcc structures are in good agreement with experimental values for the present many-body potential. The results are also in good agreement with the other theory [17].In the present model, a_{fcc} theoretical lattice parameters are very close to the experimental values. From the same table, one can also seen that in the present model the fcc-bcc energy differences are close to the obtained results from Ref. [17].

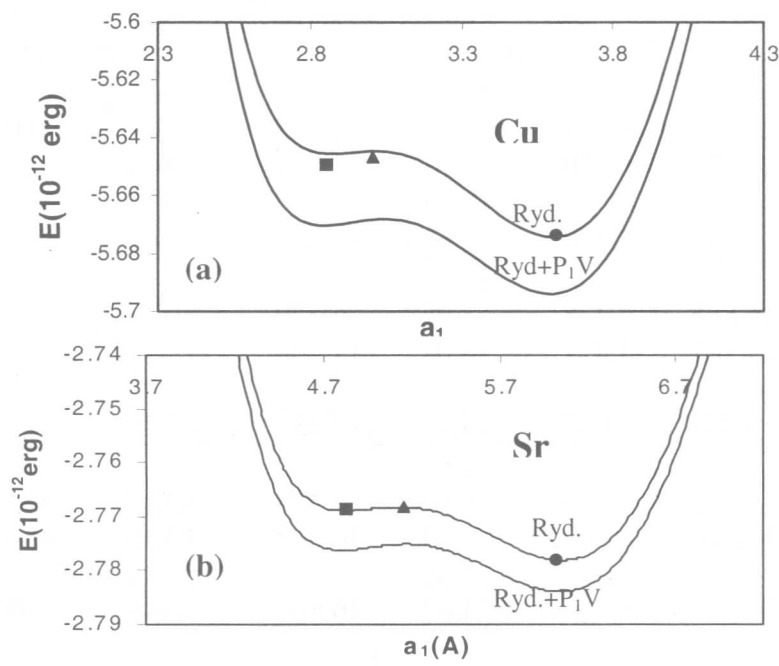


Figure 1. Dependence of the cohesive energy per atom on a_l for (a) Cu (b) Sr

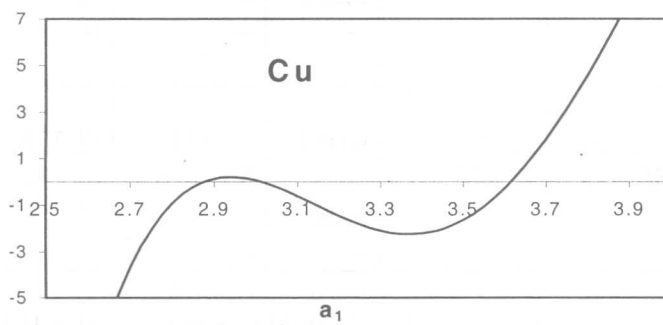


Figure 2. The applied stress σ_l as a function of a_l for (a) Cu and (b) Sr

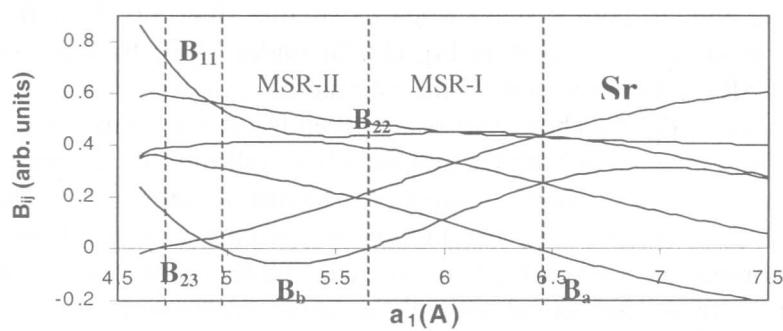


Figure 3: The variations of B_{11} , B_{22} , B_{12} , B_{23} , B_a and B_b (in arb. units) as a function of a_l for Sr

Table 2.Theoretical lattice parameters (*a*), atomic volumes (*V*) and cohesive energies (*E*) per atom of the unstressed bcc and fcc sructures for Cu, Ag, Al, Ca, and Sr

Metal	$A_{bcc}(\text{\AA})$	$V_{bcc}(\text{\AA})^3$	E_{bcc} (10^{-12} erg)	$a_{fcc}(\text{\AA})$	$V_{fcc}(\text{\AA})^3$	E_{fcc} (10^{-12} erg)	$E_{fcc}-E_{bcc}$ (10^{-12} erg)	
Cu	Ryd.	2.864	11.745	-5.645	3.671	12.367	-5.674	-0.0286
	Ryd+P ₁ V	2.874	11.872	-5.670	3.615	11.810	-5.694	-0.0236
	Exp. [18]	--	--	--	3.615	--	-5.584	--
	Ref. [17]	2.856	11.640	-5.550	3.600	11.660	-5.600	-0.0499
Ag	Ryd.	3.232	16.885	-4.778	4.068	16.829	-4.818	-0.0402
	Ryd+P ₁ V	3.249	17.161	-4.811	4.09	17.104	-4.845	-0.0333
	Exp. [18]	--	--	--	4.09	--	-4.720	--
	Ref. [17]	3.225	17.240	-4.687	4.1	17.23	-4.720	-0.0325
Al	Ryd.	3.205	16.461	-4.675	4.028	16.338	-4.818	-0.0402
	Ryd+P ₁ V	3.222	16.724	-4.7002	4.05	16.607	-4.845	-0.0333
	Exp. [18]	--	--	--	4.05	--	-5.424	--
	Ref. [17]	3.220	16.690	-5.216	4.03	16.360	-5.344	-0.0325
Ca	Ryd.	4.443	43.853	-2.634	5.473	40.984	-2.644	-0.0095
	Ryd+P ₁ V	4.468	44.612	-2.665	5.580	43.435	-2.668	-0.0035
	Exp. [18]	--	--	--	5.580	--	-2.944	--
	Ref. [17]	--	--	--	--	--	--	--
Sr	Ryd.	4.824	56.126	-2.768	6.053	55.441	-2.778	-0.0092
	Ryd+P ₁ V	4.845	56.855	-2.776	6.08	56.188	-2.784	-0.008
	Exp. [18]	--	--	--	6.08	--	-2.752	--
	Ref. [17]	--	--	--	--	--	--	--

In order to see whether the bcc phase is stable or not, we plot $B_a(=B_{22}^2-B_{23}^2)$, $B_b(=(B_{11}(B_{22}+B_{23})-2B_{12}^2))$, B_{11} , B_{22} and B_{23} as a function of cell length a_l in Fig 3 for Sr. Figure 3 shows, that in tension, when the cell length a_l is longer than in 6.424 Å, B_a becomes negative, and in compression when a_l smaller than 5.653 Å, B_b is violated. Thus, according to the criteria given in Eq. (5), Sr under [100] loading has an elastic stability region (ESR) and corresponds to the internal of variation of lattice parameter a_l between 5.653 Å and 6.424 Å. These ranges are given for metals considered in Table 3.

One can see from Fig. 2 that both fcc and bcc phase fall into the mechanical stability region (MSR). Hence, from the point of view of mechanical stability, fcc and bcc phase is stable. From Fig. 3. it seen that the failure first occurs in tension when $C_b>0$ is violated and in compression when $C_a>0$ is violated. Table 3 summarizes the values of lattice parameter a_l stress (theoretical strength) at failure in tension and in compression. Table 3 shows the MSR-I and MSR-II values for all fcc metals considered. The region of lattice stability determined from the failure criteria is shown in Fig. 3. Theoretical strengths in tension and compression are taken to be the stresses observed in Fig.2 at the

boundaries of the region of stability. Table 3 lists the values of stress σ_l calculated at failure in tension and compression. The other theoretical strength values are also given in Table 3 for the sake of compression.

Table.3 Values of cell lengths a_l in tension and in compression for Cu, Ag, Al, Ca, and Sr for stress σ_l (theoretical strength) where the Born stability criteria are violated.

Metal	MSR-I			MSR-II	
	Failure in Compr.(B_b)	Failure in Tens.(B_a)		B_{23}	B_b
	a_l (A)	a_l (A)	σ_l (GPa)	a_l (A)	a_l (A)
Cu	3.3480	3 .8402	3.2250 2.75*	2.8001	2.9298
Al	3.7526	4.2845	1.6442 1.41*	3.1166	3.2882
Ag	3.7590	4.3654	2.7806 2.41*	3.1860	3.2774
Ca	5.4550	6.4892	0.2536	4.7161	5.0110
Sr	5.6530	6.4240	0.2443	4.6700	4.9600

*: are taken from Ref. [8]

Table. 4 Second-order elastic constants C_{ij} (10^{12} dyn/cm²) at T=0K of some fcc metals

Metal	This Study						Experiment [20]		
	C_{11}^p	C_{12}^p	C_{44}^p	C_{11}^T	C_{12}^T	C_{44}^T	C_{11}	C_{12}	C_{44}
Cu	1.6376	1.1919	0.6944	1.7054	1.2205	0.7287	1.700	1.225	0.758
Ag	1.1785	0.8307	0.5087	1.2488	0.8608	0.5456	1.240	0.934	0.461
Al	0.8655	0.6429	0.3627	0.9195	0.6660	0.3910	1.143	0.619	0.316
Ca	0.2277	0.1335	0.1073	0.2969	0.1631	0.1436	0.228	0.160	0.140
Sr	0.1395	0.1047	0.0581	0.1453	0.1052	0.0618	0.153	0.103	0.099

Table 5. Third-order elastic constants (C_{ijk}) (10^{-12} dyn/cm²) of some fcc metals

C_{ijk}	Cu	Ag	Al	Ca	Sr
C_{111}^p	-10.810	-8.329	-5.627	-2.485	-8.864
C_{111}^T	-10.730	-8.238	-5.558	-2.307	-7.962
C_{111} (Exp.)	-10.400	-8.170	-5.390	--	--
C_{112}^p	-7.633	-5.798	-4.018	-1.307	-6.323
C_{112}^T	-7.609	-5.772	-3.999	-1.257	-6.074
C_{112} (Exp.)	-7.700	-5.870	-4.060	--	--
C_{123}^p	0.871	0.514	0.503	0.1289	0.8635
C_{123}^T	0.881	0.524	0.511	0.1485	0.9626
C_{123}^T (Exp.)	0.920	0.540	0.530	--	--

Experimental values are taken from [21].

Also, it can be seen from Table 4 and 5 that the computed values of SOEC and TOEC at atmospheric pressure and at $T=0$ K are in good agreement with their experimental values. Especially, TOEC are in good agreement for the present total energy. We believe that the volume dependent energy added to two-body potential improved the present results.

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