Advance Physics Letter

Lattice stability of Aluminum using two body potential in case of two directional stresses

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Abstract— Taking simple two body potential {$\Phi = -A r^{-n} + B \exp(-Pr^{m})$}, strength and stability of Aluminum are estimated in case of two directional stresses. Computed value of theoretical strength is 1.6GPa (tensile strength) at 3.88% of strain and – 28.3GPa (compressive strength) at -3.68% of strain. We compare our results with calculated results of other workers. Second phase found in tension.

Index Terms— Strength, stability, two body potential, stress, second phase

I. INTRODUCTION

We know from literature the theoretical or ideal strength of a perfect crystal is defined as the strength at which a perfect lattice becomes mechanically unstable. Since a perfect crystal is homogeneous throughout, it cannot become mechanically unstable till the system lowers its totals energy by spontaneously undergoing uniform deformations. Calculations of theoretical strength of cubic metals have been active field in research. Many applications [1] – [9] of theoretical strength and stability are presents in literature. Recently many authors [10] - [41] work on this problem in different loading conditions. Cerney and coworkers [18] - [24] studied mechanical stability of cubic metals (Ni, Ir, Fe, Cr) in hydrostatic loading and uniaxial loading using simulation technique. Based on Born- Hill- Milistein elastic stability theory Ho et al [25] investigates the effect of transverse loading on ideal tensile strength of six fcc materials using molecular statics and density function theory simulation. Mouhat et al [26] gives necessary and sufficient stability conditions for non-cubic and lower symmetry classes crystals. Ogata et al [27] gives review article on this topic.

In this paper we have calculated theoretical strength of Aluminum in two directional stresses mode of deformation by taking K D [42] and generalized Morse potential [43], [44]. Main work was done by Thakur et al (28) in this mode of deformation. Recently Zhang et al [16] and Vikram Singh [35] calculated theoretical strength of copper in this mode of deformation. In this case two forces of the equal sign (either compressive or tensile) are simultaneously applied along the a_2 and a_3 directions, while zero force applied along a_1 direction. So the approach consists in changing the lattice parameters a_2 ($=a_3$) by small amount and relaxing the value of a_1 such that the condition $F_1=0$ (force applied along a_1 direction) is satisfied.

II. COMPUTATIONAL DETAILS

Two body potential as suggested by Kuchhal and Dass [42] is given by

$$\Phi = -A r^{-n} + B \exp(-Pr^{m}) \qquad (1)$$

Where A, B and p are positive constant and are expressed in unit of erg.cm^n, erg and cm^{-m} respectively. Constant m and n are adjustable parameters and r is the distance from the lattice site with coordinate specified by the three integers l_1, l_2, l_3 are

$$r = \tfrac{1}{2} (a_1^2 l_1^2 + a_2^2 l_2^2 + a_3^2 l_3^2) \qquad (2)$$

Where l_1, l_2 and l_3 are integers (chosen such that $l_1 + l_2 + l_3$ is even for a fcc lattice) a_1, a_2 and a_3 are cell lengths of unit cell. Since this potential is empirical in nature, there is no limit to the number of different functions, which can be calculated from a given set of experimental data. Thus any family of potential function should include relatively short-range steep potential as well as longer range shallower potentials.

This potential contains two adjustable parameters m, n and three unknown potential parameters A, B and P which can be calculated by using experimental values of lattice constant, bulk modulus and cohesive energy. Table 1 gives calculated values of unknown potential parameters A, B and P of Aluminum taking cohesive energy, lattice constant and bulk modulus as an input data [45].

Adjustable parameters		Unknown parameters		
m	n	P (cm^{-m})	A(erg. cm^{n})	B (erg)
1	1/5	3.507×10^{9}	1.638×10^{-16}	7.2939×10^{26}

Table: - 1 Potential parameters

Detailed theory has been given by Milstein [43], [44] for applying Born [1] stability criteria to the determination of mechanical stability of cubic crystals in the presence of applied forces and deformations. For cubic crystals with central interactions, the necessary and sufficient conditions for a lattice to be in stable equilibrium are

$B_{12} > 0, B_{23} > 0$ (3)

$B_{22} - B_{23} > 0$ (4)

$B_{11}(B_{22} + B_{23}) - 2B_{12} > 0$ (5)

For brevity of notation we represent $\{B_{22} - B_{23}\}$ by ab1 and $\{B_{11}(B_{22} + B_{23}) - 2B_{12}\}$ by ab2.

Stress σ_i is being given by

$$\sigma_i = \frac{1}{a_j a_k}\frac{\partial E}{\partial a_i} = \frac{u}{2}\frac{a_i}{a_j a_k}\sum_{l_1}\sum_{l_2}\sum_{l_3} l_i^{\,2}\frac{\partial \Phi(r)}{\partial a_i} \quad (6)$$

Where E is the energy per unit cell

$$E = \frac{u}{2}\sum_{l_1}\sum_{l_2}\sum_{l_3}\Phi(r) \quad (7)$$

B_{ij} are given by

$$B_{ij} = \frac{\partial^2 E}{\partial a_i \partial a_j} = \frac{u}{8}\sum_{l_1}\sum_{l_2}\sum_{l_3} l_i^{\,2} l_j^{\,2}\frac{\partial^2 \Phi(r)}{(\partial r^2)^2} + \frac{u}{4}\delta_{ij}\sum_{l_1}\sum_{l_2}\sum_{l_3} l_i^{\,2}\frac{\partial \Phi(r)}{\partial r^2} \quad (8)$$

for i, j =1,2,3

Where δ_{ij} is the Kronecker delta function and u is the number of atoms per unit cell. The summations are carried out over a number of atoms sufficiently large to ensure that convergence up to four significant figures is achieved.

F_i is the force along a_i direction can also be written

$$F_i^k = F_i^s + \sum_{j=1}^{6} B_{ij}^s\left(a_j^k - a_j^s\right) \quad i = 1,2,3,4,5 \text{ and } 6 \quad \ldots(9)$$

Where F_i^s and a_i^s are the values of force and lattice constant at starting state values (which is initially supposed to equilibrium values) i.e., a_i^0 for which $F_i^s = 0$ F_i^k and a_i^k are the values of force and lattice constant at nearby state of starting state.

In the absence of applied shear stress, the components a_4, a_5 and a_6 will retain their initial values of 90° (at least up until failure occurs).

Equation (9) can be written as

$$F_1^k = F_1^s + B_{11}^s(a_1^k - a_1^s) + B_{12}^s(a_2^k - a_2^s) + B_{13}^s(a_3^k - a_3^s) \quad (9a)$$

$$F_2^k = F_2^s + B_{21}^s(a_1^k - a_1^s) + B_{22}^s(a_2^k - a_2^s) + B_{23}^s(a_3^k - a_3^s) \quad (9b)$$

$$F_3^k = F_3^s + B_{31}^s(a_1^k - a_1^s) + B_{32}^s(a_2^k - a_2^s) + B_{33}^s(a_3^k - a_3^s) \quad (9c)$$

In this case,

$a_2 = a_3$ and $F_1^k = F_1^s = 0$ (i.e. force in x- direction is absent)

We can calculate all B_{ij} from equation 8 for starting values of lattice constants ($a_1^s = a_2^s = a_3^s = a_0$). For the known values of $a_2^k(= a_3^k)$ we can calculate a_1^k from equation 9a, and using the values of a_1^k and $a_2^k(= a_3^k)$, $F_2^k(= F_3^k)$ can be calculate from equation 9b or 9c. We can further calculate B_{ij} from equation 8 for the values of $a_1^k \neq a_2^k(= a_3^k)$. If the stability condition is not violated, the set of $a_1^k \neq a_2^k(= a_3^k)$, $F_2^k(= F_3^k)$ is now suppose as $a_1^s, a_2^s(= a_3^s)$, $F_2^s(= F_2^s)$, and the same procedure follows until the any one of the stability condition is violated. Stress and strain of the set a_1, a_2 (= a_3), F_2 (=F_3) for which the stability conditions violated, gives the strength and stability of cubic metals. As mentioned previously this method were developed and applied by Thakur et al [28] – [32] for Ni and Zhang et al [16] and Vikram Singh [35] for Cu.

III. RESULTS AND DISCUSSION

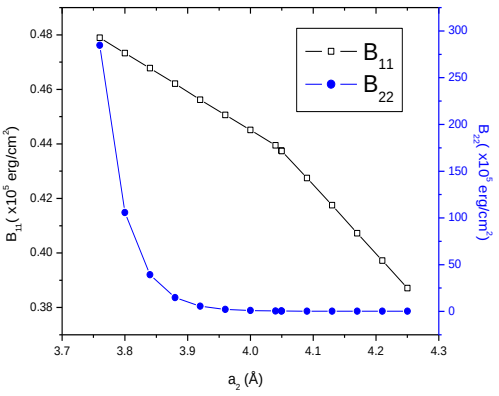

Figure 1 Variation of B_{11} and B_{22} with respect to a_2 (=a_3)

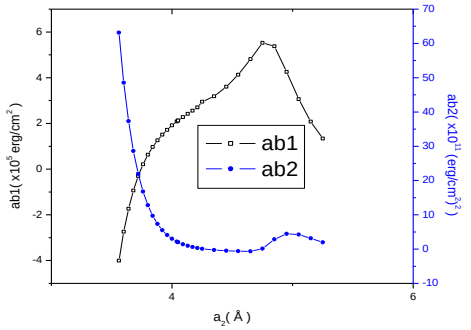

Figure 2 Variation of B_{12} and B_{23} with respect to a_2 (=a_3)

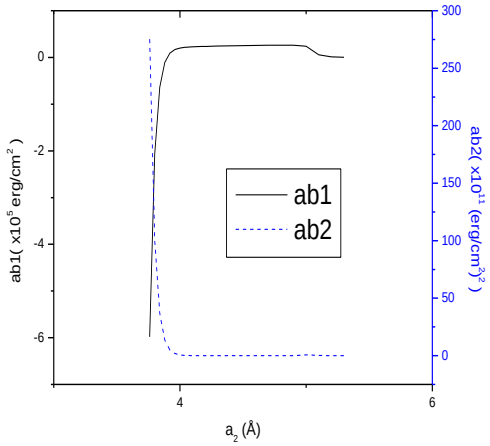

Figure 3 Variation of ab1 and ab2 with respect to a_2 (=a_3)

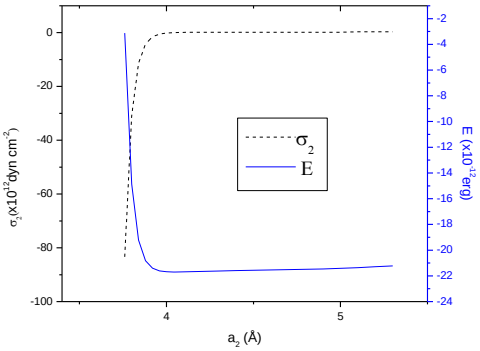

Figure 4 Variation of σ_2 (= σ_3) and energy per unit cell (E) with respect to a_2 (=a_3)

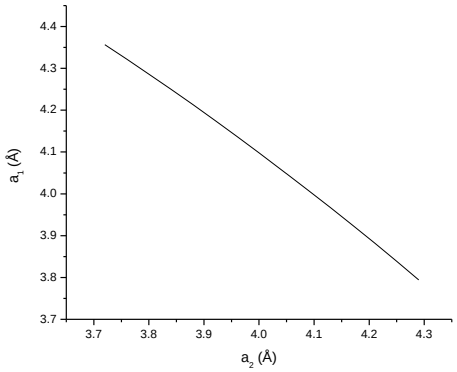

Figure 5 Variation of a_1 with respect to a_2 (=a_3)

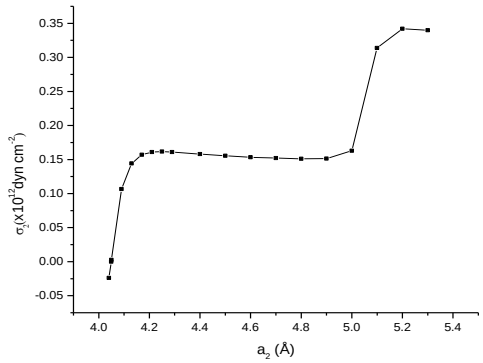

Figure 6 Variation of σ_2 (= σ_3) with respect to a_2 (=a_3)

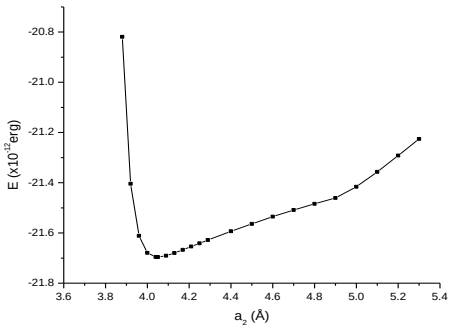

Figure 7 Variation of energy per unit cell (E) with respect to a_2 (=a_3)

Adjustable parameters		Failure in tension		Failure in compression	
m	n	a_2(=a_3) (Å)	σ_2 (=σ_3) (Gpa)	a_2(=a_3) (Å)	σ_2 (=σ_3) (Gpa)
1	1/5	4.2059	1.6	3.9	-28.3

Table 2 Strength of Aluminum in case of two directional stresses

Figure from 1 to 5 show the dependency of B_{ij}, its functions (i.e. ab1 and ab2), stress (σ_2), energy per unit cell (E) and lattice constant a_1 on a_2. Figure 6 and 7 shows the detail variation of stresses (σ_2= σ_3) and energy per unit cell (E) with respect to a_2 (=a_3) in tension. Table 2 gives the calculated values of breaking stress (i.e. theoretical strength) and lattice constant a_2 (=a_3) (at which the instability occur).

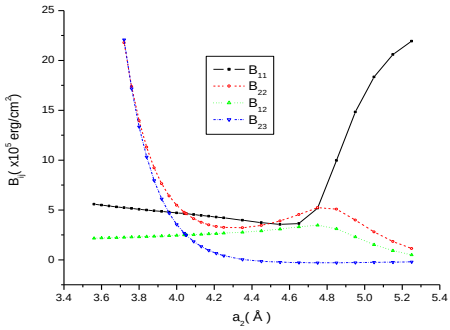

Figure 8 Variation of B_{ij} with respect to a_2 at q=6 in generalized Morse potential

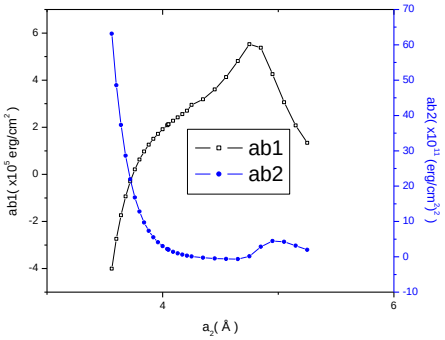

Figure 9 Variation of ab1and ab2 with respect to a_2 for q=6 in generalized Morse potential

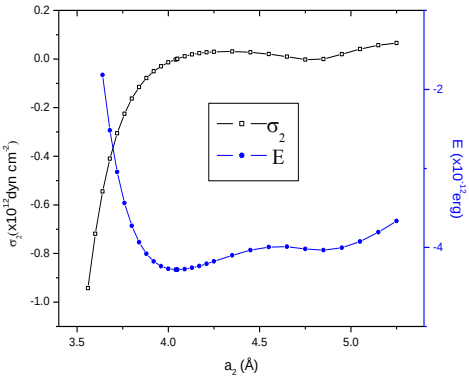

Figure 10 Variation of σ_2 and energy per unit cell (E) with respect to a_2 for q=6 in generalized Morse potential

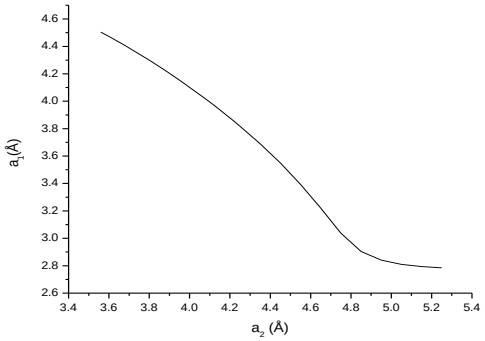

Figure 11 Variation of a_1 with respect to a_2 for q=6 in generalized Morse potential

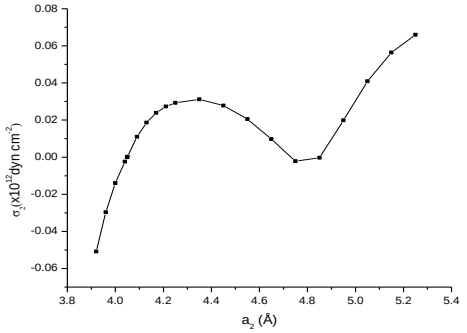

Figure 12 Variation of σ_2 with respect to a_2 for q=6 in generalized Morse potential

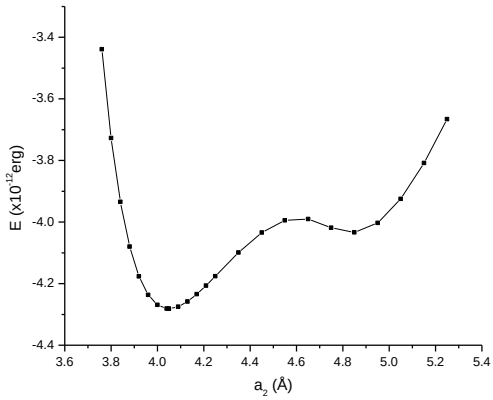

Figure 13 Variation of energy per unit cell (E) with respect to a_2 for q=6 in generalized Morse potential

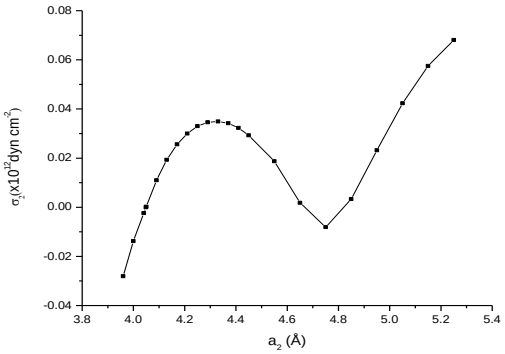

Figure 14 Variation of σ_2 with respect to a_2 for q=1.25 in generalized Morse potential

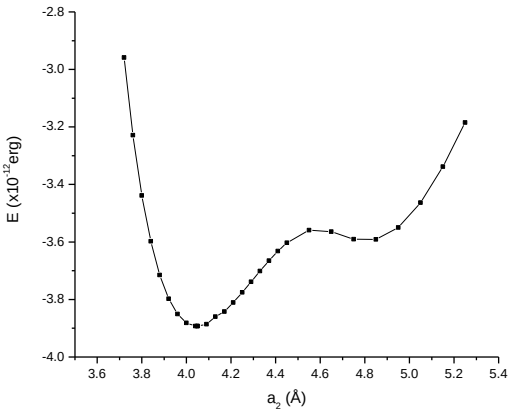

Figure 15 Variation of energy per unit cell (E) with respect to a_2 for q=1.25 in generalized Morse potential

Adjustable parameters	Failure in tension		Failure in compression	
q	$a_2(=a_3)$ (Å)	σ_2 (=σ_3) (Gpa)	$a_2(=a_3)$ (Å)	σ_2 (=σ_3) (Gpa)
1.25	4.29603	3.4643	3.71569	-21.852
2	4.2928	3.3812	3.71874	-22.725
6	4.28666	3.0316	3.74364	-25.818

Table 3 Strength of Al in case of two directional stresses for different values of q in generalized Morse potential

Figure from 8 to 11 show the variations of B_{ij}, its functions (i.e. ab1 and ab2), stresses ($\sigma_2 = \sigma_3$), energy per unit cell (E) and lattice constant a_1 with respect to a_2 for q=6 in generalized Morse potential. Figure 12 shows the detail variation of stresses ($\sigma_2 = \sigma_3$) with respect to a_2 ($=a_3$) in tension at adjustable parameter q=6 in generalized Morse potential. Figure 13 shows energy per unit cell (E) with respect to a_2 ($=a_3$) at adjustable parameter q=6 in generalized Morse potential. Similarly figure 14 and 15 shows detail variation of stresses ($\sigma_2 = \sigma_3$) and energy per unit cell (E) with respect to a_2 ($=a_3$) at q= 1.25 in generalized Morse potential. Table 3 shows the calculated values of breaking stress (i.e. theoretical strength) and lattice constant a_2 (at which the Born stability criteria violated) for different values of q in generalized Morse potential.

In tension the stability condition ($B_{23}>0$) is violated at a_2 ($=a_3$) = 4.2059 (Å) and in compression the stability condition (ab1>0) is violated at a_2 ($=a_3$) = 3.9 (Å). At these values of a_2 ($=a_3$), the stresses (breaking stresses) σ_2 ($=\sigma_3$) = 1.6 GPa at 3.88% of strain in tension and σ_2 ($=\sigma_3$) = -28.3 GPa at - 3.68% of strain in compression have been found in K D potential. Breaking stress in (100) loading [45] for same potential is 2.348GPa (in tension) and –1.994GPa (in compression). Figure 6 and figure 7 show minima in E and small dip in σ_2 ($=\sigma_3$). These results show second unstable phase during tension.

In Morse potential, the stability condition (ab2>0) is violated at a_2 ($=a_3$) = 4.28666 (Å) with stresses σ_2 ($=\sigma_3$) =3.0316 GPa in tension and the stability condition (ab1>0) is violated at a_2 ($=a_3$) =3.74364 (Å) with stresses σ_2 ($=\sigma_3$) =-25.818GPa in compression for q=6. These results show in table 3. Breaking stress in (100) loading [45] for the same potential is 6.14GPa (in tension) and –3.541 (in compression). Figure from 12 to 15 also show second phase in tension.

As per our knowledge experimental values of strength were not found in literature in this mode of deformation, so we compare our results with theoretical results of other investigators. Recently Wang et al [10], [11] calculated strength and stability of Au in uniaxial loading and hydrostatic deformation and reported 4.2GPa in uniaxial loading and 19.2GPa in hydrostatic loading. Zhang et al [15], [17] calculated strength of Au and Cu crystal in (100) loading by using EAM and found 6.31GPa for Au and 7.525GPa for Cu. Friak et al [36] have shown that the strength of copper is 29 GPa in (111) direction, 31 GPa in (110) direction and 33 GPa to 55 GPa in (001) direction. Taking MAEAM recently Zhang et al have calculated strength of Cu and found from -15.131GPa to 2.803GPa at -5.801% to 4.972% of strain in this mode of deformation [16] and 7.525GPa in (100) loading [17]. Vikram Singh [35] calculated strength of copper in this mode of deformation using K D potential and found strength – 85.83GPa (compressive) at – 3.16% of strain and 1.62GPa (tensile) at 8.57% of strain which are of the same order of magnitude as our results.

From figures 6, 12 and 14 show a dip in stresses curve in tension i.e. if we increase the lattice constant a_2, initially stresses increase and then decrease and after reaching a minimum values it again increases. Similarly figures 7, 13 and 15 show very small dip in energy per unit cell curve. So these results show that another phase exit in tension. We found from our result this phase is unstable in both type of phenomenological interaction i.e. K D and generalized Morse potential. Milstein [44] and recently Wang et al [11] reported the second phase in compression of (100) loading for fcc metals. In (100) loading, second phase exit when we decrease a_1 (due to the presence of force F_1) and increase a_2 ($=a_3$). When we compare these results with our results, the situation of a_1, a_2 ($=a_3$) are same but only difference is that this situation created by force F_1 in (100) loading and by forces F_2 ($=F_3$) in this mode of deformation i.e. in two directional stresses. So we conclude that a second phase exit in tension of this mode of deformation.

IV. CONCLUSIONS

As per our knowledge nobody can evaluate the theoretical strength and stability of aluminum in this mode of deformation. As such no experimental data is available in this mode of deformation. We compare our results with calculated results of other workers and found our results are same order of magnitude of results of other theoretical investigators. In future we calculate theoretical strength of metals using EAM as an interaction between atoms.

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