Mechanical Stability of Copper in (100) loading

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Abstract: Taking simple two body potential $\Phi = -A\ r^{-n} + B\ \exp(-Pr^{m})$, strength and stability of copper are estimated in (100) loading mode of deformation. Computed values of theoretical strength of copper is 3.2135GPa (tensile strength) at 6.20% of strain and – 2.745GPa (compressive strength) at 3.853% of strain. We compare our results with calculated results of other workers and conclude that this potential gives better results as compare to other potential.

Keywords : Strength, stability, two body potential, stress, tension.

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I. Introduction

Calculations of theoretical strength of cubic metals have been active field in research. Mechanical (theoretical) strength was defined as stress or strain at which perfect crystal lattice became mechanically unstable with respect to arbitrary deformation. Many workers [1-23] have estimated theoretical strength of cubic metals in different loading conditions. Cerney and coworkers [6-12] studied mechanical stability of some cubic metals (Ni, Ir, Fe, Cr) in hydrostatic loading and uniaxial loading using simulation technique. Based on Born- Hill- Milstein elastic stability theory, Ho et al [13] recently investigates the effect of transverse loading on ideal tensile strength of some FCC materials using molecular statics simulation and density function theory. Ogata et al [14] gave a review article on this topic. Taking EAM, few workers [15-20] calculated strength and stability of cubic metals. Recently Singh [21-23] have been calculated theoretical strength and stability of Cu and Al in various loading conditions.
In this paper, we calculate theoretical strength of Copper in (100) loading by taking simple two body potential which is developed by Kuchhal et al [24] and recently used by Singh [21-23]. This potential contains two adjustable and three unknown parameters which are calculated by taking experimental values of some physical quantity. By taking experimental values of lattice parameter and second order elastic constant, Kuchhal et al [24] have been calculated unknown parameters for some BCC metals and by taking experimental values of lattice parameter, bulk modulus and cohesive energy, Singh [22-23] calculated unknown parameters for Copper and Aluminum. In this study, section I gives present status of the work, section II gives two body potential and stability conditions in (100) loading, section III gives results and discussion of the work, section IV gives conclusions of the work and the last section V gives references of the work.

II. Theory and Procedure

The two body potential as suggested by Kuchhal and Dass [24] is given as

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

Where A, B and P are positive constants and are expressed in unit of $erg.cm^{n}$, erg. and cm^{-m} respectively. r is the distance from a lattice site chosen as the origin to a given lattice site with coordinate specified by the three integers $l_1.l_2, l_3$ as

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

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. Since this potential is basically empirical one 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. The selection of adjustable parameters m and n are such that the calculated value of strength and stability are close with experimental results. Further, the potential parameters A, B and P are determined by using the experimental values of lattice constant, bulk modulus and cohesive energy keeping m and n as adjustable parameters.

Singh et al [22-23] gave a method for determination of potential parameters A, B and P in this potential for FCC metals by taking lattice constant, cohesive energy and bulk modulus as an input data. These parameters are shown in table 1.

m	n	P (cm^{-m})	A ($erg.cm^{n}$)	B (erg)
1	1/24	$24.498x10^{9}$	$1.2622\ x10^{-15}$	$5.5836x10^{255}$
1	1/5	$5.135x\ 10^{9}$	$1.0715\ x10^{-16}$	$1.4563x10^{42}$
1	1	$1.0598x10^{9}$	$4.0143x10^{-22}$	.0208
3	1	$5.818x10^{23}$	$4.0035\ x10^{-22}$	$5.508x10^{-10}$

Table 1: Calculated unknown potential parameters for different values of adjustable parameters m and n.

Determination of mechanical stability of cubic crystals in the presence of applied forces and deformations, the detailed theory has been given by Milstein [17]. In case of (100) loading mode of deformation, Singh [23] recently calculated strength and stability of Aluminum. Since detailed mathematical equations and theory are present in this paper [23], so we are not further repeat here.

The necessary and sufficient conditions for a lattice to be in stable equilibrium are:

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

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

III. Results and discussion

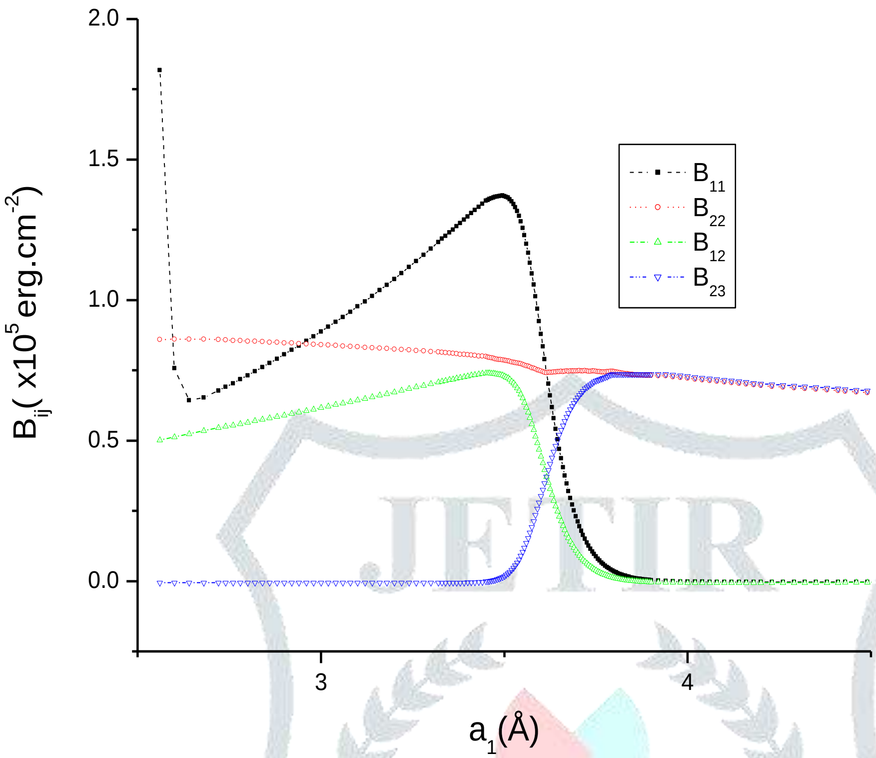

Figure 1: Variation of B_{ij} with respect to lattice constant a_1 for m=1and n=1/5

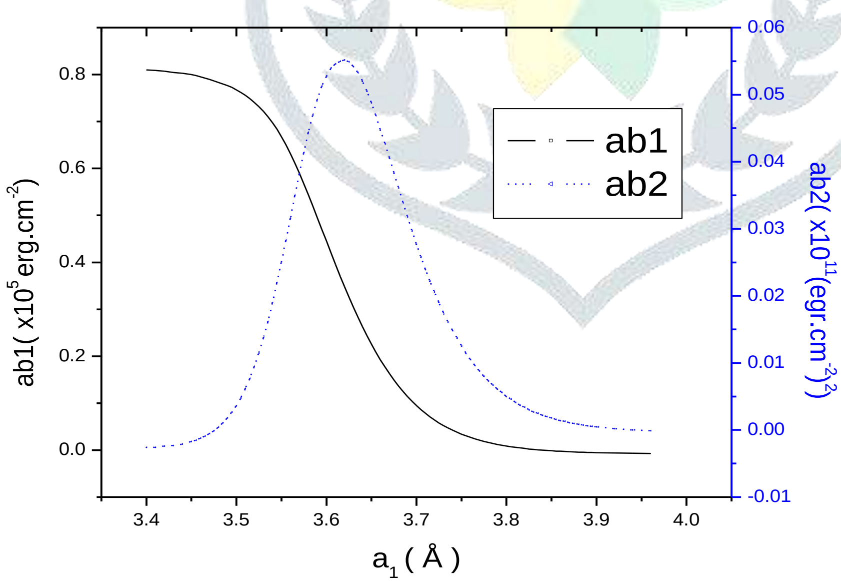

Figure 2: Variation of ab1 and ab2 with respect to a_1 for m=1and n=1/5

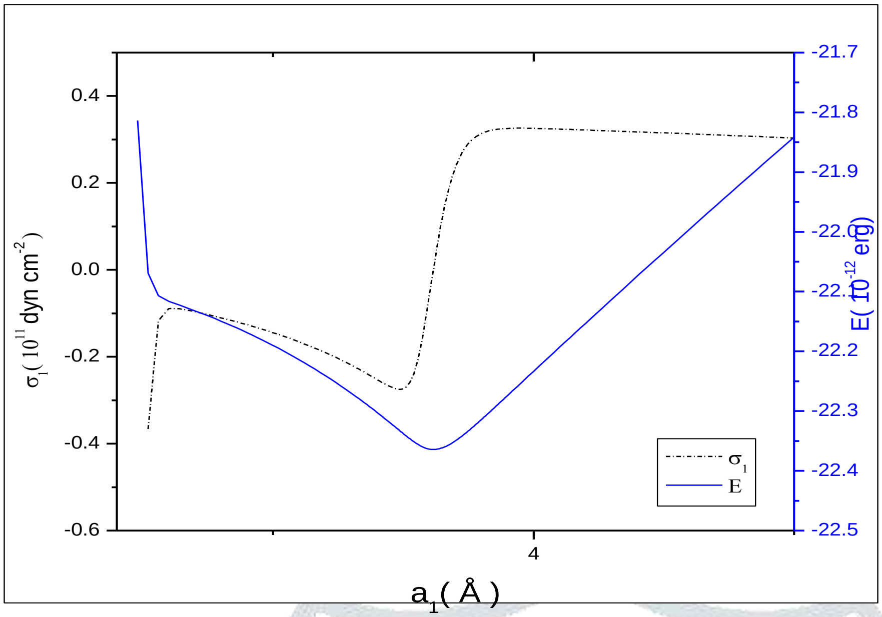

Figure 3: Variation of stress (σ_1) and energy per unit cell (E) with respect to a_1 for m=1and n=1/5.

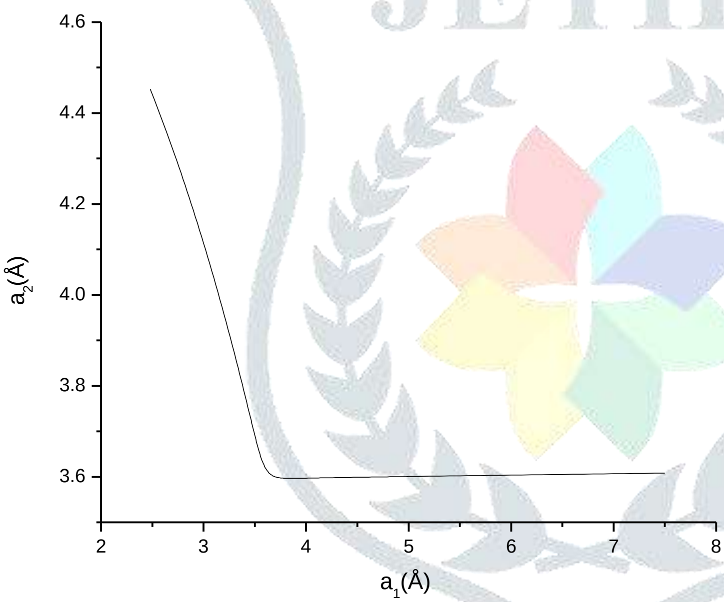

Figure 4: Variation of (a_2) with respect to a_1 for m=1and n=1/5.

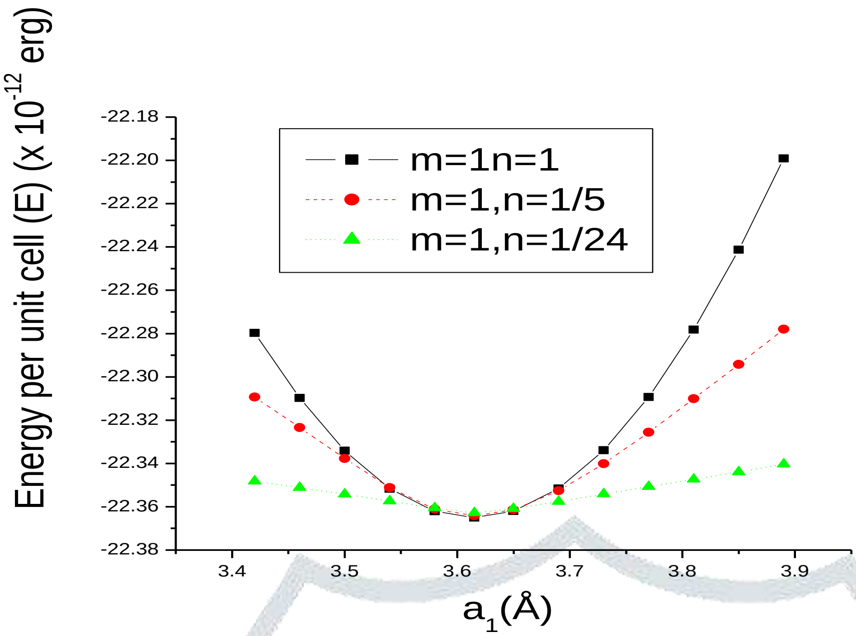

Figure 5: Variation of energy per unit cell (E) with respect to a_1 for fixed values of adjustable parameter m=1, and different value of adjustable parameter n

Adjustable parameter		Failure in tension		Failure in compression	
m	n	a_1(Å)	σ_1(GPa)	a_1(Å)	σ_1(GPa)
1	1/24	3.6811	.78	3.5759	-.79
1	1/5	3.83945	3.214	3.47611	-2.745
1	1	4.1478	13.63	3.208	-8.38
3	1	4.15074	14.0554	3.2032	-8.602

Table 2: Breaking stress of copper for different values of adjustable parameter and n in K.D. potential

Figure 1 and 2 show the variation of B_{ij} and it's functions (i.e. ab1 and ab2) with respect to lattice constant a_1 for the fixed values of adjustable parameter m=1 and n=1/5. Variation of stress (σ_1) and energy per unit cell (E) are shown in figure 3 for the same fixed value of adjustable parameter m=1 and n=1/5. Figure 4 shows the variation of lattice constant a_2 with respect to lattice constant a_1 for the fixed value of adjustable parameter m=1 and n=1/5. The variation of energy per unit cell (E) with respect to a_1 are shown in figure 5 for the different values of n and fixed value of m=1. Table 3 gives the calculated values of breaking stress (i.e. theoretical strength) and lattice constant a_1 at which the stability condition is violated at different values of adjustable parameters m and n. From these results, theoretical strength in (100) loading are very close with experiments when the values of m = 1 and n = 1/5. From figures 1 and 2, when we increases a_1, ab_1=0 (i.e. Born stability criteria violated) at a_1= 3.83945Å and when we decreases lattice constant a_1, ab_2=0 (Again stability condition violets) at a_1= 3.476Å. From figure 3, at a_1= 3.83945 the breaking stress (σ_1) is equal to 32.135x10^9 dyn/cm^2 (3.2135 GPA), and at a_1=3.476 (Å), breaking stress (σ_1) is equal to -27.45x10^9 dyn/cm^2 (-2.745 GPA). These results give tensile and compressive strength of copper in (100) loading. So the theoretical strength (tensile strength) of copper is 3.2135 GPa at 6.20% of strain (i.e. stability) and compressive strength is equal to -2.745GPa at 3.853% of strain. To calculate theoretical strength which were close with experimental value we select different sets of adjustable parameters m and n. Table 3 gives the calculated values of breaking stress in tension as well as in compression for different values of m and n. From this table, breaking stress in tension is equal to .78 GPa at n =1/24 (for fixed value of m=1), is equal to 13.63 GPa at n=1 (for fixed value of m=1), is equal to 14.0554 GPa at m=3 (for fixed value of n=1) and is equal to 13.63 GPa at m=1 (for fixed value of n=1). So from these results we conclude that breaking stress highly depends on adjustable parameter n and less depends on adjustable parameter m. As we see in figure 5 that the parameter n changes the breadth of potential. From this figure, if we decrease the value of adjustable parameter n, the breadth of potential increases, so we conclude that the breaking stress is the function of breadth of potential. We can compare our result with Morse type of interaction between atoms. By using Morse potential, Milstein [25] have been calculated theoretical strength of copper and found 6.97GPa which is approximate two time of experimental result 2.94 GPa [26]. Singh [21] also calculated theoretical strength in this mode of deformation by taking highly complicate energy per unit cell calculation (pseudo potential calculation) and found out the value .125GPa which is very low in comparison to experimental value. By using K D potential we can find out the value of breaking stress very low which tend to the value evaluated by Singh [21] by taking pseudo potential, moderate value which tend to the experimental value and high value which tend to the value evaluated by Milstein et al [25]. Some other investigators also calculated theoretical strength of copper by taking EAM as an interaction between atoms. Milstein et al [19] calculated this as 9.8 GPa, Cifti et al [16] calculate this as 5.279 GPa, Cai et al [28] calculated this as 3.3 GPa and recently Zhang et al [17] calculated this as 7.522GPa by using EAM approach.

IV Conclusion

This study show that the two body K.D. potential gives better results in comparison to other type of interactions. This study also shows that the theoretical strength is highly potential dependent. Further, from above discussion our calculated results are very close with experimental results in comparison to calculated results of other investigators. Few differences between experimental results and our results exit due to presence of dislocation and imperfection in the experimental specimen.

V. **References**

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