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Strength and Stability of Copper Using Simple Two Body Potential

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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 case of two directional stresses. Computed values of theoretical strength of copper is 1.62GPa (tensile strength) and – 85.83GPa (compressive strength). We compare our results with calculated results of other workers. Second phase found in tension.***

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

1. Introduction

Calculations of theoretical strength of cubic metals have been active field in research. The ideal (theoretical) strength was originally defined as stress or strain at which perfect crystal lattice became mechanically unstable with respect to arbitrary homogeneous infinitesimal deformation. Many applications of theoretical strength [1-18] and stability are presents in literature. Recently many authors [19-50] are working on this problem in different loading conditions. Cerney and coworkers [27-33] 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 [34] investigates the effect of transverse loading on ideal tensile strength of six fcc materials using molecular statics and density function theory simulation. Mouhat [35] et al gives necessary and sufficient stability conditions for non-cubic and lower symmetry classes crystals. Ogata et al [36] gives review article on this topic.

In this paper we evaluated theoretical strength of fcc copper when two forces of same sign (either compressive or tensile) are simultaneously applied along the a_2 and a_3 directions {i.e. $F_2=F_3$}, while zero force is applied along the a_1 direction {i.e. $F_1=0$}. This method was developed by Thakur et al [37] and calculated strength and stability of many cubic metals in this mode of deformations. Zhang et al [25] have calculated strength and stability of copper in this mode of deformation by using MAEAM. This type of deformation is named by Thakur et al [37] as two directional stresses. In this mode of deformation we calculate theoretical strength of copper by taking simple two body potential.

2. Computational Details

Two body potential as suggested by Kuchhal and Dass [51] is given by

$$\phi = -Ar^{-n} + B\, exp(-Pr^{m}) \quad (1)$$

Where A, B and P are positive constant and are expressed in unit of erg.cm^n, erg and cm^{-m} respectively. 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

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

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 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 as an input data. The selection of adjustable parameters m and n are such that the calculated value of theoretical strength are close with experimental results. Table 1 gives calculated values of unknown potential parameters A, B and P of copper taking cohesive energy, lattice constant and bulk modulus as an input data [50]. Here we take adjustable parameters m =1 and n=1/5, since this potential gave the strength in (100) loading which are close with experimental results.

Table 1: Potential parameters of copper

Adjustable parameters		Unknown parameters		
m	n	P (cm^{-m})	A(erg. cm^n)	B (erg)
1	1/5	5.135×10^{9}	1.0715×10^{-16}	1.4563×10^{42}

Detailed theory has been given by Milstein [53] 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

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

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

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

For brevity of notation we represent $\{B_{22} - B_{23}\}$ by ab1 and $\{B_{11}(B_{22} + B_{23}) - 2\,B_{12}\}$ 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 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 (12) 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 mode of deformation $a_2 = a_3$ 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 $a_1^s = a_2^s = a_3^s = a_0$. 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 $a_1^k \neq a_2^k(= a_3^k)$ and $F_2^k(= F_3^k)$ is now suppose as $a_1^s, a_2^s(= a_3^s)$ and $F_2^s(= F_3^s)$, 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) and 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 [37-41] for many metals and recently by Zhang et al [25] for copper.

3. Results and Discussion

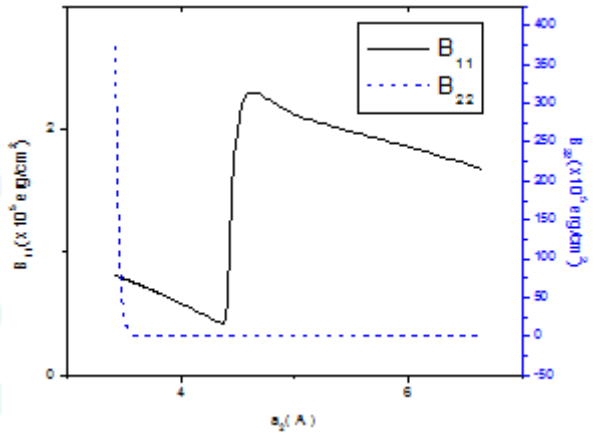

Figure 1: Variation of B_{11} and B_{22} with respect to a_2 (=a_3)

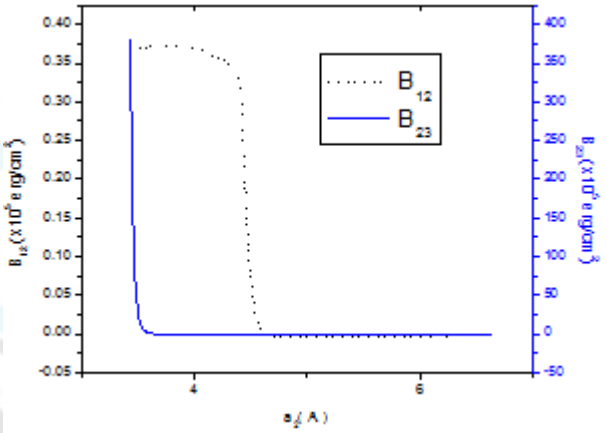

Figure 2: Variation of B_{12} and B_{23} with respect to a_2 (=a_3)

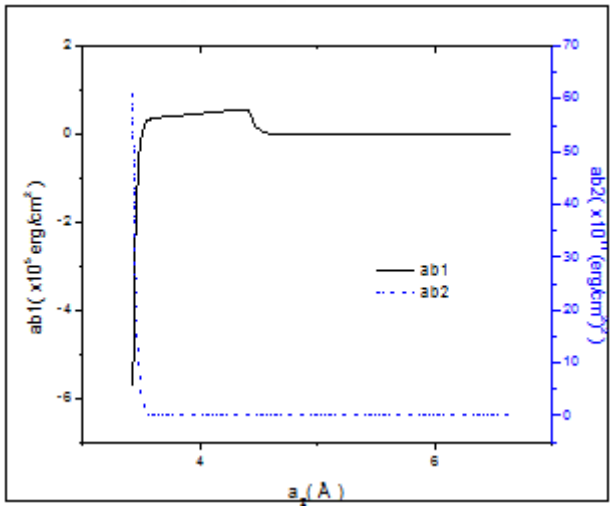

Figure 3: Variation of ab1 and ab2 with respect to a_2 (=a_3)

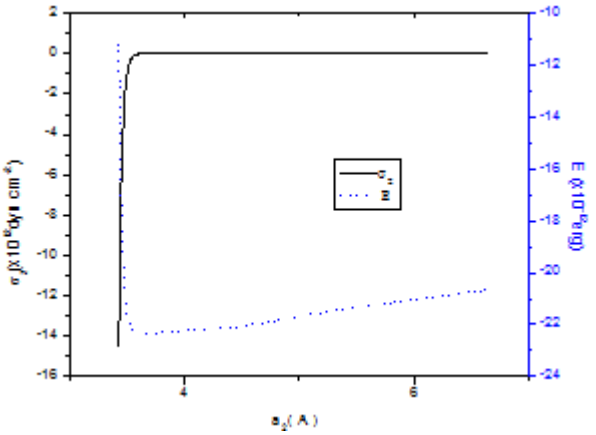

Figure 4: Variation of σ_2 (=σ_3) and energy per unit cell (E) with respect to a_2 (=a_3)

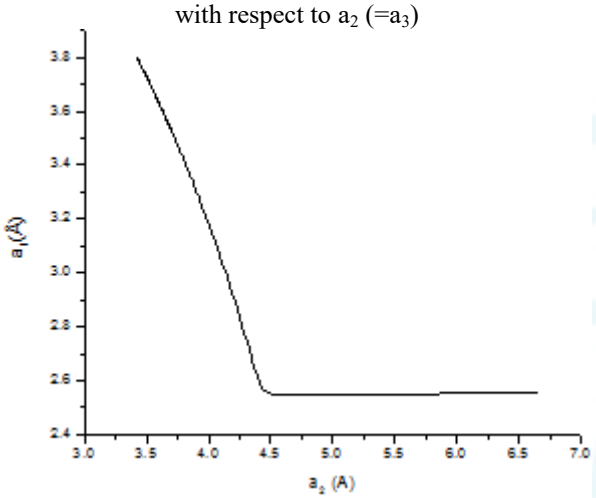

Figure 5: Variation of a_1 with respect to a_2 (=a_3)

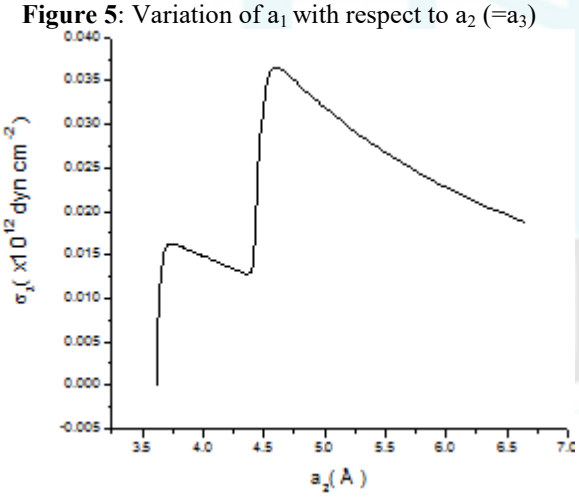

Figure 6: Variation of σ_2 (=σ_3) with respect to a_2 (=a_3)

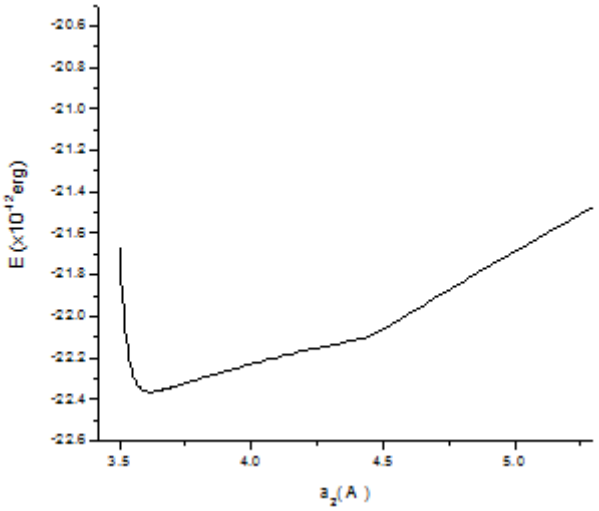

Figure 7: Variation of energy per unit cell (E) with respect to a_2 (=a_3)

Table 2: Strength of copper in case of two directional stresses

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	3.9252	1.62	3.50224	-85.83

Variations of B_{ij}, it's functions (i.e. ab1 and ab2), stresses (σ_2= σ_3), energy per unit cell (E) and lattice constant a_1 with respect to a_2 (=a_3) are shown in figure from 1 to 5 for fixed values of adjustable parameters m=1 and n=1/5 in K.D. potential. Figure 6 and 7 show the detail variation of stresses σ_2 (= σ_3) and energy per unit cell of copper at m=1 and n=1/5. Table 2 gives the calculated values of breaking stresses (i.e. theoretical strength) and lattice constant a_2 (=a_3) at which the instability occur of copper for different values of adjustable parameter m and n.

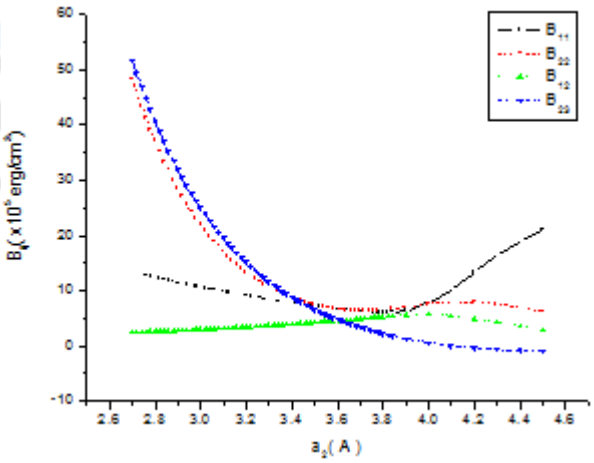

Figure 8: Variation of B_{ij} with respect to a_2 (=a_3) for q=6 in generalized Morse potential

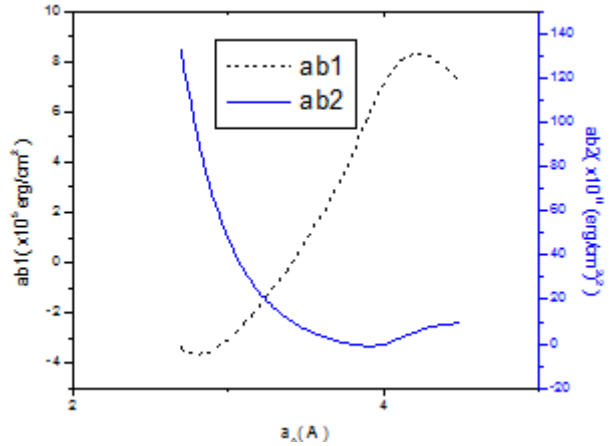

Figure 9: Variation of ab1 and ab2 with respect to a_2 (=a_3) for q=6 in generalized Morse potential

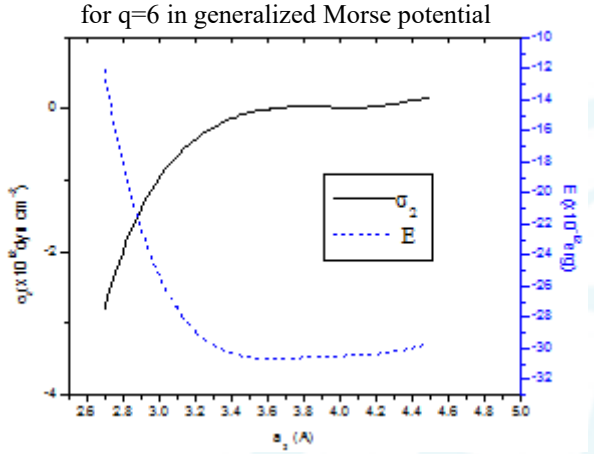

Figure 10: Variation of σ_2 (= σ_3) and energy per unit cell (E) with respect to a_2 (=a_3) for q=6 in generalized Morse potential

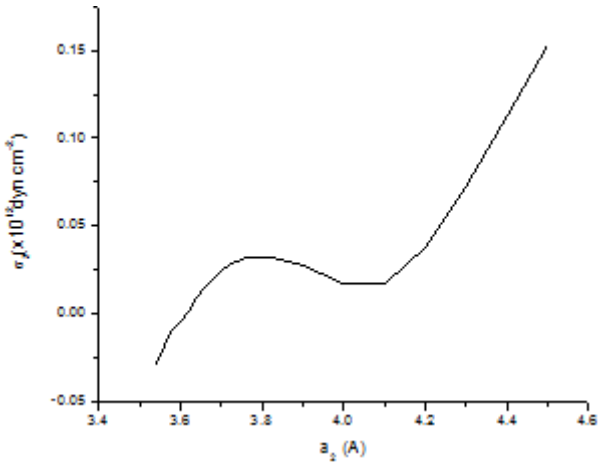

Figure 12: Variation of σ_2 (= σ_3) with respect to a_2 (=a_3) for q=6 in generalized Morse potential

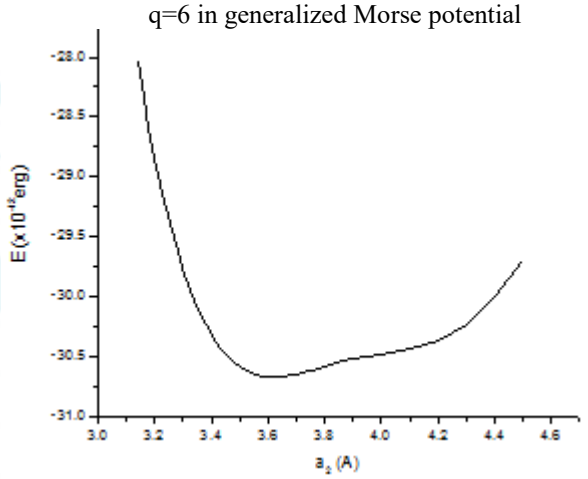

Figure 13: Variation of energy per unit cell (E) with respect to a_2 (=a_3) for q=6 in generalized Morse potential

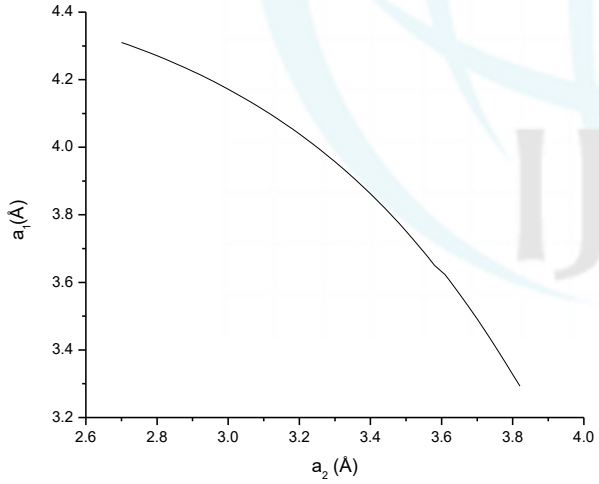

Figure 11: Variation of a_1 with respect to a_2 (=a_3) for q=6 in generalized Morse potential for copper

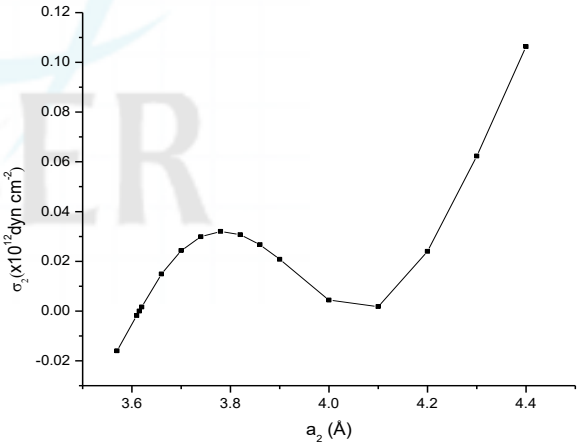

Figure 14: Variation of σ_2 (= σ_3) with respect to a_2 (=a_3) for q=1.25 in generalized Morse potential

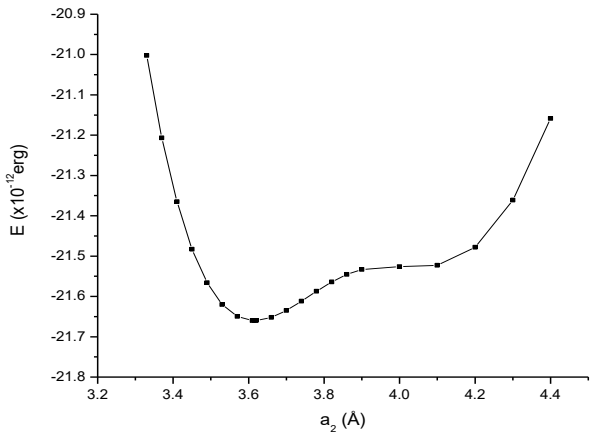

Figure 15: Variation of energy per unit cell (E) with respect to a_2 (=a_3) for q=1.25 in generalized Morse potential

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

Adjustable parameter	Failure in tension		Failure in compression	
q	a_2 (=a_2) (Å)	σ_2 (=σ_2) (Gpa)	a_2 (=a_2) (Å)	σ_2 (=σ_2) (Gpa)
1.25	3.76108	3.101	3.44839	-8.656
2	3.76135	3.0965	3.44773	-8.7256
6	3.780942	3.25094	3.410242	-12.4568

We can compare our calculated results of K D potential with results of generalized Morse potential. So we calculate theoretical strength of copper by taking generalized Morse potential as an interaction between atoms. Figure from 8 to 11 show the variations of B_{ij}, it's functions (i.e. ab1 and ab2), stresses (σ_2= σ_3), energy per unit cell (E) and lattice constant a_1 of copper with respect to a_2 (=a_3) for q=6 in generalized Morse potential. Figure 12 and 13 show the detail variation of stresses (σ_2= σ_3) and energy per unit cell (E) of copper with respect to a_2 (=a_3) for q=6 in generalized Morse potential. Figure 14 and 15 show the detail variation of stresses (σ_2= σ_3) and energy per unit cell (E) of copper with respect to a_2 (=a_3) for q=1.25 in generalized Morse potential. Table 3 gives the calculated values of breaking stresses (i.e. theoretical strength) and lattice constant a_2 (=a_3) at which the instability occur of copper for different values of adjustable parameter q in generalized Morse potential.

We can point out from these figure the variation of B_{ij}, it's functions (i.e. ab1 and ab2), stresses (σ_2= σ_3), energy per unit cell (E) in both potential are similar. Same type of variation of stresses σ_2 (=σ_3) and energy per unit cell (E) of Ni with respect to lattice constant a_2 (=a_3) were find by Thakur et al (36). For K D potential (m=1, n=1/5), when we increase a_2 (=a_3) the stability condition (B_{23}>0) violated at a_2 (=a_3) = 3.9252 (Å) and similarly when we decrease a_2 (=a_3) the condition (ab1>0) violated at a_2(=a_3) = 3.50224 (Å). At a_2(=a_3) =3.9252 (Å), the breaking stresses (tensile strength) is equal to 1.62GPa. Similarly at a_2(=a_3) =-3.50224 (Å) the breaking stresses (compressive strength) = -85.83 GPa. These values give theoretical strength 1.62 GPa (in tension) at 8.57% of strain and -85.83 GPa (in compression) at - 3.13% of strain. The strength of copper in case of unidirectional stress {(100) loading} is calculated and equal to 3.215GPa.

In generalized Morse potential the stability condition ab_1>0 is violated at a_2 (=a_3) = 3.78094 (Å) in tension and the stability condition ab_2>0 is violated at a_2 (=a_3) = 3.41024 (Å) in compression. The breaking stresses at these points are σ_2 (=σ_3) = 3.2509GPa (in tension) and σ_2 (=σ_3) = -12.457GPa (in compression). These values give the theoretical strength 3.2509 GPa in tension at 4.58% of strain and -12.457 GPa in compression at - 5.67% of strain. Table 3 shows calculated values of breaking stress for different values of adjustable parameter q in generalized Morse type of interaction between atoms. We conclude from these results that breaking stresses decrease in tension and compression if we increase adjustable parameter q in generalized Morse potential. In K D potential figures 6, 7 show a minima in stress and minima in energy per unit cell in tension which shows the second phase in tension. Figure 12-15 gives the similar results in case of Morse potentials.

As per our knowledge the experimental values of strength in this case of deformation were not available in literature, so we compare our calculated results with theoretical results of Cu [25] and Ni [37]. Zhang et al have calculated the strength of copper from -15.131GPa to 2.803GPa at strain -5.801% to 4.972% in this mode of deformation taking MAEAM [25] and 7.525GPa in (100) loading [26]. The calculated value of Nickel is 6 GPa [37] when two directional stresses are applied and is 15.55GPa [54] when unidirectional stress {i.e. (100) loading} is applied. Thus from these result the strength in case of unidirectional stress is approximately 2 times the strength in case of two directional stresses. In our case we too are getting the same 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. Milstein [54] and recently Wang et al [20] reported the second phase in compression of (100) loading for fcc metals. In (100) loading this second phase exit, when we decrease a_1 and a_2 (=a_3) increase due to the presence of force F_1 (i.e. the force in x direction). 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. Zhang et al [25] also reported same second unstable phase for copper.

4. Conclusions

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 in magnitude of results of other theoretical investigators. Zhang et al [25] calculated strength and stability of copper in this mode of deformation using MAEAM. We know that the calculations in pair potential are simple in comparison to EAM. So our analysis is simple in comparison to Zhang et al.

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