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Strength and Stability of Copper in (100) Loading using EAM

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Abstract

Numerical computations of strength and stability of copper in case of (100) loading are carried out by taking new embedded atom method (EAM). New EAM contains three adjustable parameters and four unknown parameters, which have calculated using experimental values of lattice constant, second order elastic constants. Computed value of theoretical strength of Cu is same order in magnitude of the results of other investigators. Second unstable phase found in compression.

Keywords: *Strength, stability, EAM, stress*

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INTRODUCTION

Calculations of theoretical strength of cubic metals have been active field in research. Many workers have been calculated theoretical strength of cubic metals in various modes of deformations by taking various types of interaction between atoms [1–16]. 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 this problem are presents in literature. Cerney and coworkers studied mechanical stability of cubic metals (Ni, Ir, Fe, Cr) in hydrostatic loading and uniaxial loading using simulation technique [17–23]. Based on Born-Hill-Milstein elastic stability theory Ho et al. investigates the effect of transverse loading on ideal tensile strength of six FCC materials using molecular statics and density function theory simulation [24]. Recently Mouhat et al. gives necessary and sufficient stability conditions for noncubic and lower symmetry classes crystals and Ogata et al. gives review article on this topic [25, 26].

Recently by taking embedded atom method (EAM), many workers have estimated theoretical strength and stability of cubic metal in various loading conditions [1–5]. In this paper, we developed new EAM which contain three adjustable parameters and four unknown parameters. Potential parameters of this EAM have been calculated using experimental values of lattice constant and second order elastic constants as an input data. We have estimated strength of Cu in (100) loading using this analytic EAM.

EMBEDDED ATOM METHOD

The original method was subsequently expended by Bakes to treat solids with highly directional distributions of valance electron densities that is, covalent bonding, allowing for much more wider scope of applications [27]. The fundamentals of the method have been discussed in the literature in detail (see for example review [28]), so only some important aspects necessary for discussion of the present work will be given here. In the EAM format, the cohesive energy per atom E_a of a homogeneous monatomic crystal can be written as

$$E_a = \mathrm{F}(\rho) + \frac{1}{2}\sum \emptyset(r_{ij}) \quad (1)$$

With

$$\rho = \sum f(r_{ij}) \quad (2)$$

where, $F(\rho)$ is the embedded function, ρ is the total electron density at the reference atomic site, $f(r_{ij})$ is the electron density function, $\emptyset(r_{ij})$ is the pair potential function, and r_{ij} is the distance between atoms i and j. From review of literature, we conclude that many type of functions have been used for $\emptyset(r)$, $f(r)$ and

$F(\rho)$. Here, we have used generalized Morse potential function for pair interaction,

$$\emptyset(r) = \frac{D}{(q-1)}[\exp\{-q\alpha(r-r_0)\} - qexp\{-\alpha(r-r_0)\}] \quad (3)$$

$$F(\rho) = -G\,\rho^e = Gu_i, \quad (4)$$

for embedded energy and $f(r) = \frac{1}{r^s}$ for density function.

In these functions q, e, and s are adjustable parameters and D, α, r_0, and G are unknown potential parameters, which can be evaluated by taking the experimental values of lattice constant a_0 and second order elastic constants C_{11}, C_{12}, and C_{44}. Since in this EAM, three adjustable parameters q, s and e are present. So by taking different values of these adjustable parameters we can found deeper long-range potential and shallower short-range potential.

Potential Parameters

Force at equilibrium gives

$$G = -\frac{1}{2}\left[\frac{W1}{W2}\right]_{at\ a=a_0} \quad (5)$$

Where

$$W1 = \sum_{l_1,l_2,l_3} L_0\,\emptyset'$$

$$W2 = u_i' \sum_{l_1,l_2,l_3} L_0\,f'$$

$$u_i' = -e\rho^{(e-1)}$$

$$L_0 = (l_1^2 + l_2^2 + l_3^2)$$

Where prime on potential and density function represent differentiation of function with respect to r^2. However, the prime on embedded function shows the differentiation of function with respect to density function (ρ).

We can write equation of second order elastic constant C_{11}, C_{12} and C_{44} in simplified form as

$$C_{11} = AX_1 + BX_2 \quad (6)$$

Where,

$$X_1 = \frac{ua_0}{8}\left[\left(\sum_{l_1,l_2,l_3} l_1^4\,\phi_{11}''\right) - \left(u_i'\sum_{l_1,l_2,l_3} L_0\,f'\right)^{-1}\left(\sum_{l_1,l_2,l_3} L_0\,\phi_{11}'\right)R\right] \quad (7)$$

$$X_2 = \frac{ua_0}{8}\left[\left(\sum_{l_1,l_2,l_3} l_1^4\,\phi_{12}''\right) - \left(u_i'\sum_{l_1,l_2,l_3} L_0\,f'\right)^{-1}\left(\sum_{l_1,l_2,l_3} L_0\,\phi_{12}'\right)R\right] \quad (8)$$

With

$$R = u_i''\left(\sum_{l_1,l_2,l_3} l_1^2\,f'\right)^2 + u_i'\left(\sum_{l_1,l_2,l_3} l_1^4\,f''\right) \quad (9)$$

$$C_{12} = AX_3 + BX_4 \quad (10)$$

Where

$$X_3 = \frac{ua_0}{8}\left[\left(\sum_{l_1,l_2,l_3} l_1^2 l_2^2\,\phi_{11}''\right) - \left(u_i'\sum_{l_1,l_2,l_3} L_0\,f'\right)^{-1}\left(\sum_{l_1,l_2,l_3} L_0\,\phi_{11}'\right)S\right] \quad (11)$$

$$X_4 = \frac{ua_0}{8}\left[\left(\sum_{l_1,l_2,l_3} l_1^2 l_2^2\,\phi_{12}''\right) - \left(u_i'\sum_{l_1,l_2,l_3} L_0\,f'\right)^{-1}\left(\sum_{l_1,l_2,l_3} L_0\,\phi_{12}'\right)S\right] \quad (12)$$

With

$$S = u_i''\left(\sum_{l_1,l_2,l_3} l_1^2\,f'\right)\left(\sum_{l_1,l_2,l_3} l_2^2\,f'\right) + u_i'\left(\sum_{l_1,l_2,l_3} l_1^2 l_2^2\,f''\right) \quad (13)$$

$$C_{44} = AX_5 + BX_6 \quad (14)$$

Where

$$X_5 = \frac{ua_0}{8}\left[\left(\sum_{l_1,l_2,l_3} l_2^2 l_3^2\,\phi_{11}''\right) - \left(\sum_{l_1,l_2,l_3} L_0\,f'\right)^{-1}\left(\sum_{l_1,l_2,l_3} L_0\,\phi_{11}'\right)T\right] \quad (15)$$

$$X_6 = \frac{ua_0}{8}\left[\left(\sum_{l_1,l_2,l_3} l_2^2 l_3^2\,\phi_{12}''\right) - \left(\sum_{l_1,l_2,l_3} L_0\,f'\right)^{-1}\left(\sum_{l_1,l_2,l_3} L_0\,\phi_{12}'\right)T\right] \quad (16)$$

With

$$T = \left(\sum_{l_1,l_2,l_3} l_2^2 l_3^2\,f''\right) \quad (17)$$

Where

$$A = \frac{D}{(q-1)}[\exp(q\alpha r_0)],$$

$$B = \frac{Dq}{(q-1)}[\exp(\alpha r_0)]$$

$$\phi_{11}(r) = \exp(-q\alpha r)$$

and

$$\phi_{12}(r) = -\exp(-\alpha r)$$

Using simple mathematics, we can write,

$$r_0 = \frac{1}{\alpha(q-1)}\ log\left[\frac{q(C_{44}X_4 - C_{12}X_6)}{(C_{12}X_5 - C_{44}X_3)}\right] \quad (18)$$

and

$$D = \frac{(q-1)C_{12}}{\{\exp(q\alpha r_0)X_3 + q\exp(\alpha r_0)X_4\}} \quad (19)$$

where, u shows, number of atoms per unit cell. For the known value of α, evaluate X_1, X_2, X_3, X_4, X_5 and X_6 from Eqs. (7), (8), (11), (12), (15) and (16) and then calculate r_0 and D with the help of Eqs. (18) and (19). If the value of

α, r_0 and D satisfied equation of C_{11} (i.e., Eq. (6) then these values of α, r_0 and D are the solution of Eqs. (6), (10) and (14). But if these values are not satisfied Eq. (6) then take another value of known α, the same procedure follows until Eq. (6) is satisfied for the values of α, r_0 and D, which is the required solution of Eqs. (6), (10) and (14). By using these values of α, r_0 and D, we can evaluate G from Eq. (5).

The selection of adjustable parameters are such that the potential gives the accurate value of theoretical strength (i.e., calculated value of strength is close with experimental result). Table 1 gives experimental values of lattice constant (a_0) and second order elastic constants of Copper as an input data [29]. In this process the cut off distance is taken to be r_{cut} = 1.65 a_0 as used by Cifti et al. [2].

Table 1: *Input Data for Copper.*

Lattice constant	C_{11} (x10^{12} dyne/cm^2)	C_{12} (x10^{12} dyne/cm^2)	C_{44} (x10^{12} dyne/cm^2)
3.6153 Å	1.762	1.249	.818

Stability Criteria

Stability condition in EAM framework (as mentioned by Cifti et al. [2]).

$B_{55} > 0$

$B_{44} > 0$

$B_{22} > 0$

$B_{23} > 0$

$(B_{22}^2 - B_{23}^2) > 0$

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

Where, $B_{ij} = \frac{\partial^2 E}{\partial a_i \partial a_j}$

For the brevity of notation $(B_{22}^2 - B_{23}^2)$ and $B_{22}(B_{22} + B_{23}) - 2(B_{12})^2$ be supposed as ab3 and ab2, respectively.

By using simple mathematics, we can write all F_i and all B_{ij} as [2, 30, 31];

$$F_i = \frac{u a_i}{a_j a_k}\left[F'\{\sum l_i^2 f'\} + \frac{1}{2}\sum l_i^2 \phi'\right]$$

$$B_{11} = u\left[\frac{a_1^2}{4}F"\{\sum l_1^2 f'\}^2 + \frac{a_1^2}{4}F'\{\sum l_1^4 f"\} + \frac{1}{2}F'\{\sum l_1^2 f'\} + \frac{a_1^2}{8}\{\sum l_1^4 \phi"\} + \frac{1}{4}\{\sum l_1^2 \phi'\}\right]$$

$$B_{22} = u\left[\frac{a_2^2}{4}F"\{\sum l_2^2 f'\}^2 + \frac{a_2^2}{4}F'\{\sum l_2^4 f"\} + \frac{1}{2}F'\{\sum l_2^2 f'\} + \frac{a_2^2}{8}\{\sum l_2^4 \phi"\} + \frac{1}{4}\{\sum l_2^2 \phi'\}\right]$$

$$B_{12} = u\left[\frac{a_1 a_2}{4}F"\{\sum l_1^2 f'\}\{\sum l_2^2 f'\} + \frac{a_1 a_2}{4}F'\{\sum l_1^2 l_2^2 f"\} + \frac{a_1 a_2}{8}\{\sum l_1^2 l_2^2 \phi"\}\right]$$

$$B_{23} = u\left[\frac{a_2 a_3}{4}F"\{\sum l_2^2 f'\}\{\sum l_3^2 f'\} + \frac{a_2 a_3}{4}F'\{\sum l_2^2 l_3^2 f"\} + \frac{a_2 a_3}{8}\{\sum l_2^2 l_3^2 \phi"\}\right]$$

$$B_{44} = \frac{u\, a_2{}^2 a_3{}^2}{4}\left[F'\{\sum l_2^2 l_3^2 f"\} + \frac{1}{2}\{\sum l_2^2 l_3^2 \phi"\}\right]$$

$$B_{55} = \frac{u\, a_1{}^2 a_3{}^2}{4}\left[F'\{\sum l_1^2 l_3^2 f"\} + \frac{1}{2}\{\sum l_1^2 l_3^2 \phi"\}\right]$$

In all these equations

$$F' = \frac{\partial F}{\partial \rho}, F'' = \frac{\partial^2 F}{\partial \rho^2}, f' = \frac{\partial f}{\partial r^2}, f'' = \frac{\partial^2 f}{\partial (r^2)^2}, \phi' = \frac{\partial \phi}{\partial r^2} \text{ and } \phi'' = \frac{\partial^2 \phi}{\partial (r^2)^2}$$

Summations are performed over l_1, l_2, and l_3, which all are integer subject to the condition that $l_1 + l_2 + l_3$ is even for a FCC lattice. In this process same cut off distance is taken as used by Cifti et al. [2]. In (100) loading mode of deformation, uniaxial force applied perpendicular to a cube face, parallel to say the edge a_1. So for a tensile force, the edge a_1 will elongate and the edges a_2 and a_3 will contract; by symmetry it is seen that the relation a_2=a_3 will be maintained. This method developed by Milstein and used by many workers in different loading condition. [1–5, 31–33].

RESULTS AND DISCUSSION

Figures 1 to 3 show effect of adjustable parameters on energy per unit cell. From these figures, we can say that for the fixed values of s and e, if we increase q the breadth of potential increases and depth of potential also increases. Further, by increasing the adjustable parameter s (for fixed value of adjustable parameter q and e) the breadth of potential decreases and depth of potential also decreases. If we increase the adjustable parameter e (for fixed values of q and s), slight change occurs in breadth and depth of the potential.

Table 2: *Calculated Potential Parameters of Cu for Different Values of Adjustable Parameters q, s and e.*

Adjustable parameters			**Unknown parameters**			
q	s	e	α	$D(x10^{-13})$	$r_0(x10^{-8})$	G
2	10	1/20	$2.065x10^{8}$	2.1104	2.7228	$1.3605\ x10^{-15}$
2	10	1/5	$2.0725x10^{8}$	2.0329	2.7377	$1.1329\ x10^{-27}$
2	15	½	$2.249\ x10^{8}$	2.2571	2.7054	$2.6784\ x10^{-70}$
2	18	½	$2.3194x10^{8}$	2.3911	2.6797	$7.6111\ x10^{-82}$
2	3	½	$9.475\ x10^{7}$	1.3875	3.9009	$1.7594\ x10^{-23}$
2	4	1/5	$8.874x10^{7}$	3.5775	3.5352	$8.482\ x10^{-18}$
2	4	½	$8.842\ x10^{7}$	3.1575	3.1575	$1.7707\ x10^{-27}$
6	4	1/5	$5.106\ x10^{7}$	1.747	3.4331	$8.482\ x10^{-18}$
6	10	½	$5.535\ x10^{7}$	3.6354	3.1718	$5.7049\ x10^{-51}$

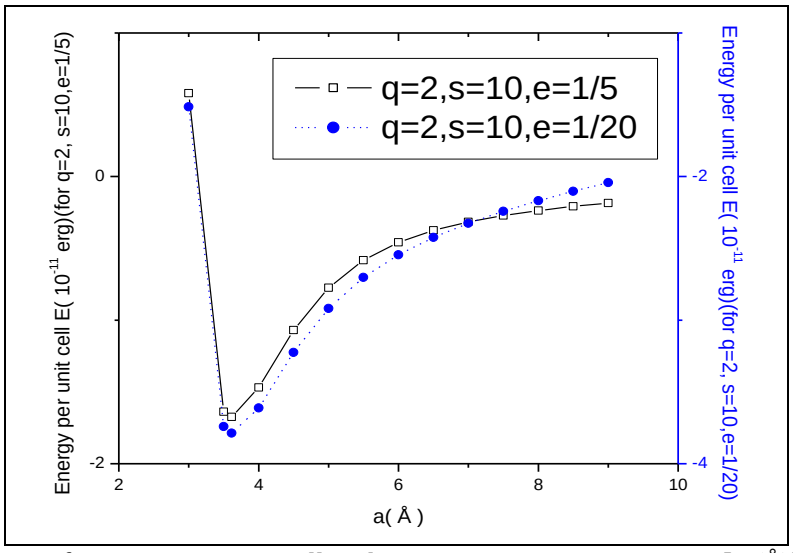

Fig. 1: *Variation of Energy per Unit Cell with Respect to Lattice Constant [a (Å)] for Different Values of Adjustable Parameters q, s and e.*

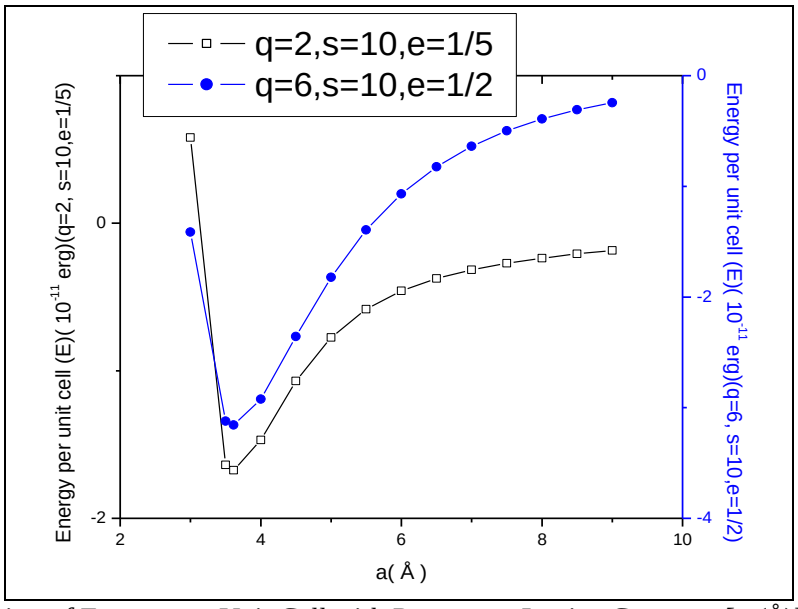

Fig. 2: *Variation of Energy per Unit Cell with Respect to Lattice Constant [a (Å)] for Different Values of Adjustable Parameters q, s and e.*

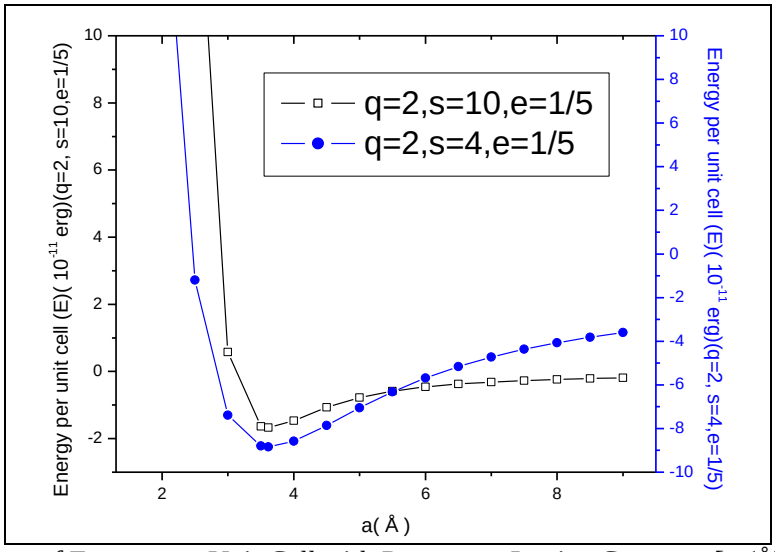

Fig. 3: *Variation of Energy per Unit Cell with Respect to Lattice Constant [a (Å)] for Different Values of Adjustable Parameters q, s and e.*

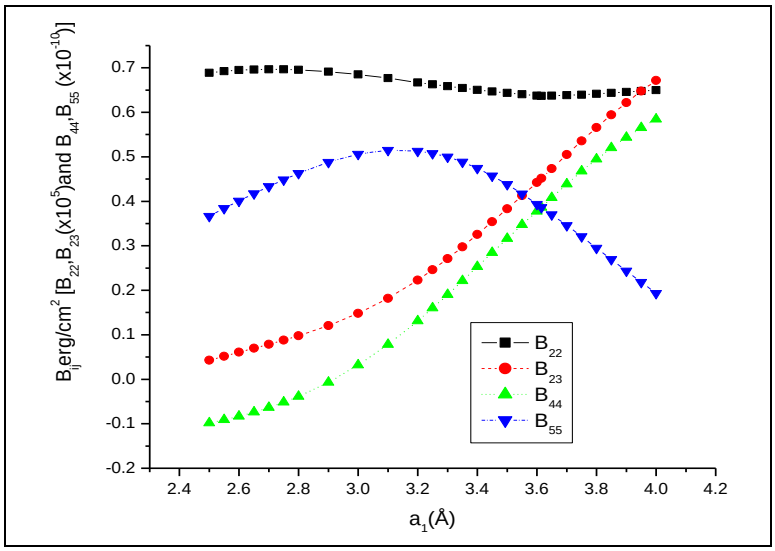

Fig. 4: *Variation of B_{ij} with Respect to a_1 for q=2, s=10 and e=1/5*

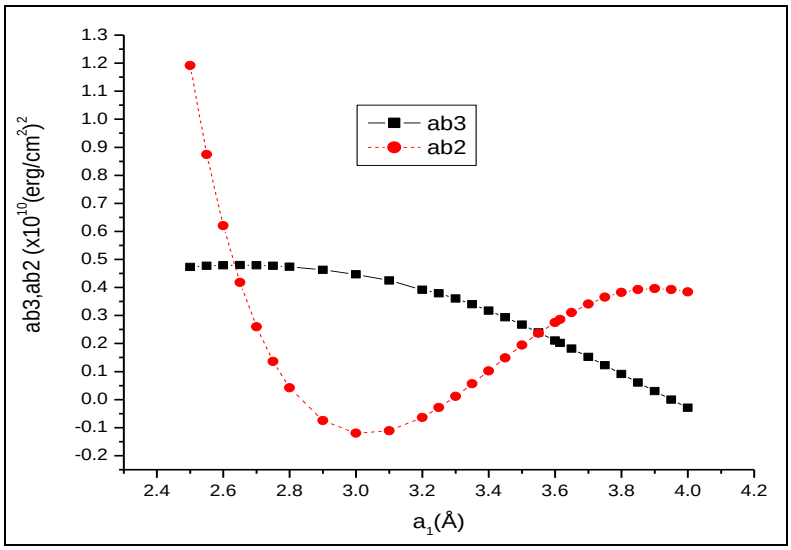

Fig. 5: *Variation of ab3, ab2 with Respect to a_1 for q=2, s=10 and e=1/5.*

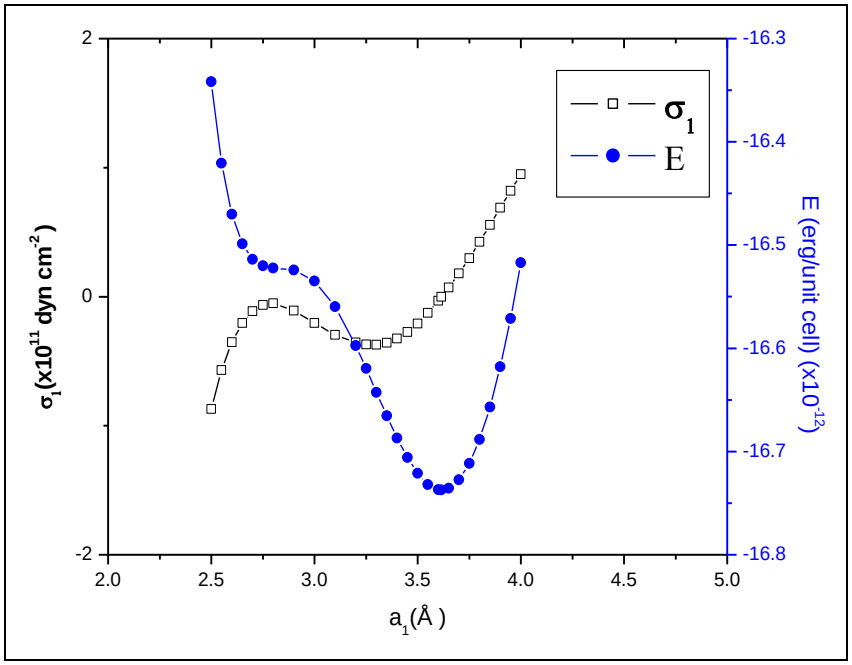

Fig. 6: *Variation of σ_1 and Energy per Unit Cell(E) with Respect to a_1 for q=2, s=10 and e=1/5.*

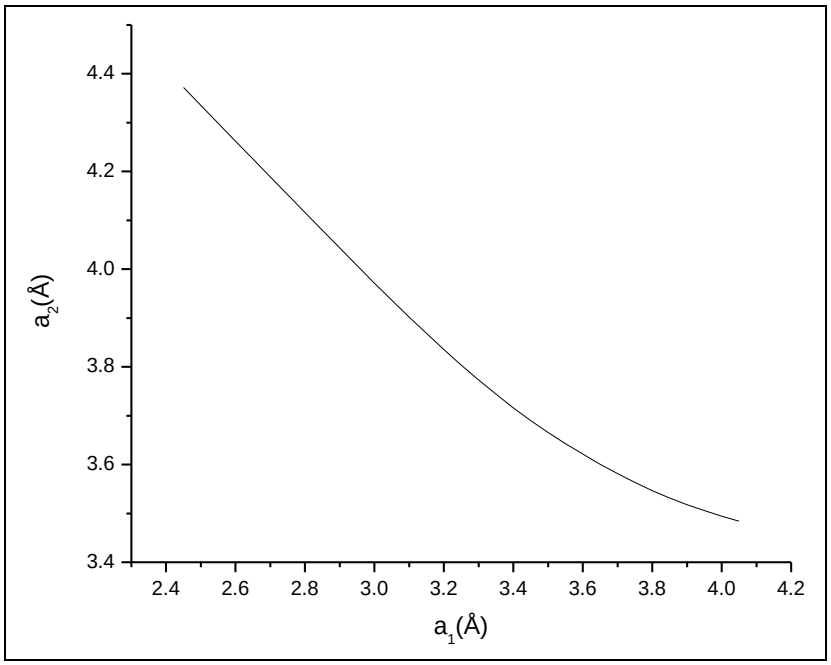

Fig. 7: *Variation of a_2 with Respect to a_1 for q=2, s=10 and e=1/5.*

Table 3: *Strength of Copper in case of 100 Loading for Different Values of Adjustable Parameters q, s and e.*

Adjustable parameters			**Failure in tension**		**Failure in compression**	
q	S	e	a_1(Å)	σ_1(Gpa)	a_1(Å)	σ_1(Gpa)
2	18	1/2	3.9701	8.623	3.28175	-3.809
6	10	1/2	4.3942	19.75	2.3452	-39.19
2	10	1/5	3.95	8.204	3.2853	-3.725
2	10	1/20	3.9498	8.202	3.2815	-3.7286

Figures 4 to 7 show the variation of B_{ij}, its functions (i.e., ab3 and ab2), stress (σ_1), energy per unit cell (E) and lattice constant (a_2) of Cu with respect to a_1 for fixed values of adjustable parameters q=2, s=10 and e=1/5. Table 3 represents breaking stress (theoretical strength) and a_1 {at which the instability occur} of copper for different values of adjustable parameters q, s and e.

When q=2, s=10 and e=1/5, Figures 5 and 6 show that the stability condition ab3>0 is violated at a_1=3.95 Å with stress σ_1= 8.204 GPa in tension and the stability condition ab2>0 is violated at a_1 = 3.285 Å with stress σ_1= -3.725 GPa in compression. These results give theoretical strength 8.204 GPa at 9.26% of strain in tension and -3.725 GPa at 9.14% of strain. This value of theoretical strength is slightly higher than experimental results but is same order of magnitude. Table 3 shows the calculated values of breaking stress in tension as well as in compression for different values of adjustable parameters q, s and e. At a_1 =2.8 Å the stress is maximum (σ_1=-.506 GPa) and energy is minimum which shows second unstable phase. Other investigators have calculated theoretical strength recently by using EAM approach. [34].

Milstein et. al. calculated this as 9.8 GPa, Cifti et al. calculated this as 5.279 GPa, Cai et al. calculated this as 3.3 GPa and recently Zhang et al. calculated this as 7.522 GPa by using EAM approach which are approximately same order of magnitude as our results [1, 2, 4, 34]. Difference between experimental results 2.94 GPa and our results exit due to presence of dislocation and imperfection in the experimental specimen wire [35].

CONCLUSIONS

We developed new analytic EAM for cubic metals, which contains only four unknown potential parameters. Method for evaluation of these potential parameters is simple. Due to presence of dislocation and imperfection in the experimental specimen wire, ideal strength of Cu is not close to experimental results. Our results are same order in magnitude of results of other workers.

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