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Strength and Stability of Al in (100) loading using EAM

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Abstract- Numerical computations of strength and stability of Aluminum in case of (100) loading are carried out by taking new analytic Embedded Atom Method (EAM). Computed value of theoretical strength of Aluminum is 9.216 GPa in tension and -38.657 GPa in compression which is same order in magnitude of the results of other investigators. Second phase is not found in compression.

Keywords- Strength, stability, EAM, stress, stability criteria.

I. INTRODUCTION

In recent years, calculations of theoretical strength of cubic metals have been active field in research. Many workers [1-17] have been calculated theoretical strength of cubic metals in various modes of deformations by taking various types of interaction between atoms. As we know 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 present in literature. 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- Milstein elastic stability theory Ho et al [25] investigated the effect of transverse loading on ideal tensile strength of six fcc materials using molecular statics and density function theory simulation. Recently Singh [26] have calculated strength of Cu using simple two body potential. Ogata et al [27] give review article on this topic. Zou et al [28] showed that a nano crystalline alloy retains an extra ordinary high yield strength over 5 GPa up to 600^0C. Ho et al [29] have investigated ideal strength of some fcc nano structures using MS simulation. Yang et al [30] have investigated ideal strength of various MC (M = Ti, Zr, Hf) systems using first principal calculations.

By taking Embedded atom method, recently many workers [1-5] have estimated theoretical strength and stability of cubic metal in various loading conditions. In most of cases, the number of unknown potential parameters is very high in these EAM. In this paper we calculated strength of Al in (100) loading mode of deformation by taking EAM, which is developed by Singh et al [17]. This EAM contains three adjustable parameters and four unknown parameters which are calculated by taking experimental values of lattice constant and second order elastic constants. In this study, section I gives present status of the work, section II gives brief idea of EAM, section III gives stability conditions in case of EAM, section IV gives results and discussion of the work, section V gives conclusions of the work and section VI gives references of the work.

II. EMBEDDED ATOM METHOD (EAM)

The original method was subsequently expended by Baskes [31] to treat solids with highly directional distributions of valance electron densities that is, covalent bonding, allowing for much more wider scope of applications. The fundamentals of the method have been discussed in the literature in detail (see for example review [32]), so only some important aspects necessary for discussion of the present work will be given here. In the EAM format, [33-35] the cohesive energy per atom E_a of a homogeneous monatomic crystal can be written as

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

With

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

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 , $\phi(r_{ij})$ 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 $\phi(r)$, $f(r)$ and $F(\rho)$. Singh et al [17] are used generalized Morse potential function for pair interaction,

$$\phi(r) = \frac{D}{(q-1)}\lfloor exp\{-q\alpha(r-r_0)\} - q\, exp\{-\alpha(r-r_0)\}\rfloor$$

$$F(\rho) = -G\rho^e$$

for embedded energy and

$f(\rho) = \frac{1}{r^s}$ 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 have been calculated by taking the experimental values of lattice constant a_0 and second order elastic constants C_{11}, C_{12}, and C_{44}.

By taking different values of adjustable parameters q, e and s, we can found deeper long range potential and shallower short range potential. Recently potential parameters D, α, r_0, and G of Cu have been calculated by Singh et al [17], by taking experimental values of lattice constant and second order elastic constants. By using the same procedure we have calculated potential parameters of Al which are shown in table 1.

Table 1 Calculated potential parameters of Al for different values of adjustable parameters q, s and e.

Adjustable parameters			Unknown parameters			
q	s	e	α(10^7 cm^{-1})	D(10^{-13} erg)	r_0(10^{-8} cm)	G (erg)
2	2	1/30	3.819	2.6834	5.6098	9.8391x10^{-11}
2	2	1/5	3.916	2.3008	5.7801	3.4238 x10^{-14}
2	15	1/5	4.6975	5.7048	4.4607	1.7937 x10^{-35}
6	15	1/5	2.1605	7.8955	4.39038	1.7937 x10^{-35}

III. STABILITY CRITERIA

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

$$B_{55} > 0$$
$$B_{44} > 0$$
$$B_{22} > 0$$
$$B_{23} > 0$$
$$(B_{22}^2 - B_{23}^2) > 0$$
$$B_{22}(B_{22} - B_{23}) - 2B_{12}^2 > 0$$

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 $B_{22}(B_{22} - B_{23}) - 2B_{12}^2$ be supposed as ab3 and ab2 respectively. Taking same analytic EAM, recently Singh et al [17] have calculated theoretical strength of Cu in (100) loading. Detailed mathematical equations and procedure of (100) loading mode of deformation are present in literature (for example see reference [17]).

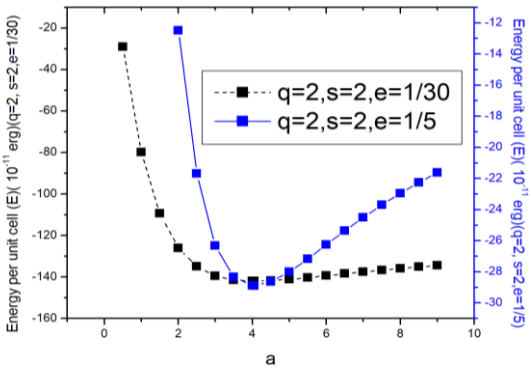

Figure 1 Variation of energy per unit cell with respect to lattice constant a (Å) for different values of adjustable parameters q, s & e.

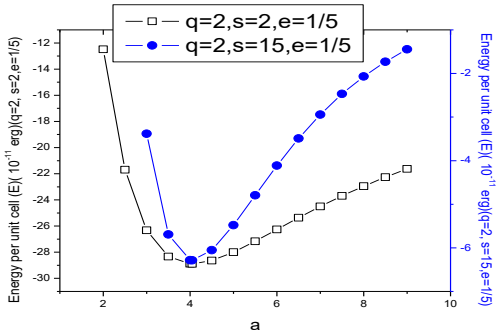

Figure 2 Variation of energy per unit cell with respect to lattice constant a (Å) for different values of adjustable parameters q, s & e.

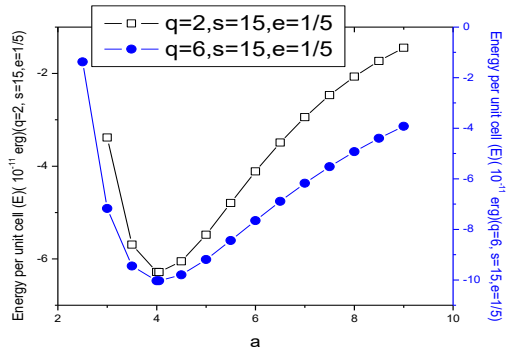

Figure 3 Variation of energy per unit cell with respect to lattice constant a (Å) for different values of adjustable parameters q, s & e.

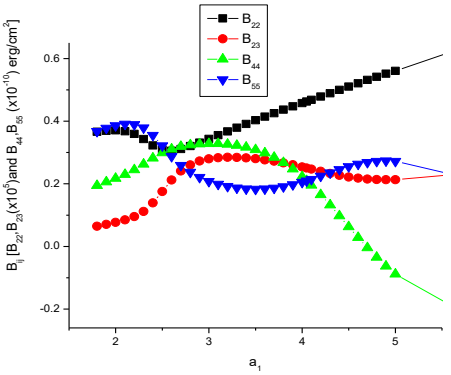

Figure 4 Variation of B_{ij} with respect to a_1 (Å) for q=2, s=15 and e=1/5.

IV. RESULTS AND DISCUSSION

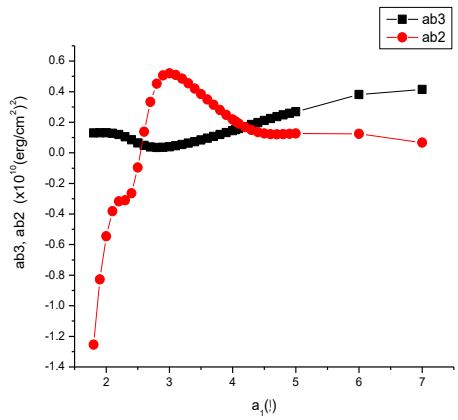

Figure 5 Variation of ab3 and ab2 with respect to a_1 (Å) for q=2, s=15 and e=1/5.

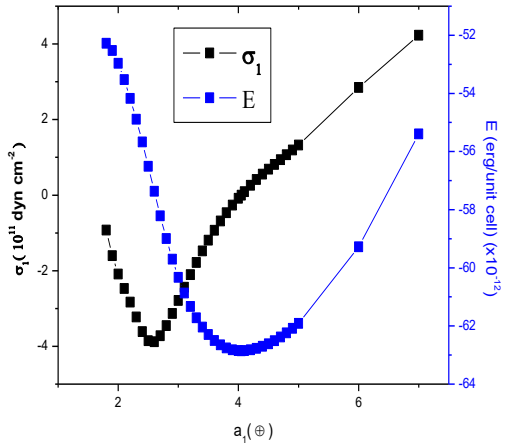

Figure 6 Variation of σ_1 and energy per unit cell (E) with respect to a_1 (Å) for q=2, s=15 and e=1/5.

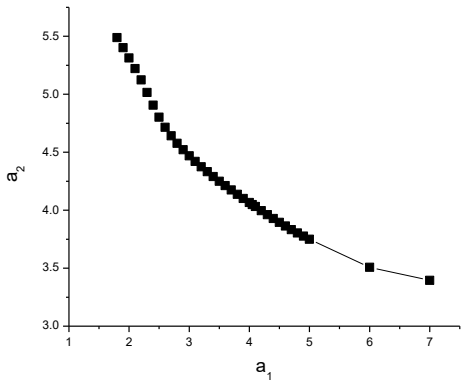

Figure 7 Variation of a_2 (Å) with respect to a_1 (Å) for q=2, s=15 and e=1/5 .

Figure from 1 to 3 show the variation of energy per unit cell (E) with respect to lattice constant a (Å) for different values of adjustable parameters q, s and e.

Figure from 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) with respect to a_1 (Å) for fixed values of adjustable parameters q=2, s=15 and e=1/5.

From figure 4 to 7, stability condition $B_{44}>0$ is violated at a_1=4.6863 (Å) with stress σ_1 = 9.216 GPa in tension and stability condition ab2 > 0 is violated at a_1= 2.55014 (Å) with stress σ_1 = - 38.657 GPa in compression. These values of stress and strain give the theoretical strength and stability of aluminum. These results show that theoretical strength is 9.216 GPa in tension and - 38.657 GPa in compression and similarly the range of stability is 15.74% in tension and 37.02% in compression. Table 2 shows the breaking stress for different values of adjustable parameters q, s and e. It is very interesting that no second phase is found in compression which was found in case of generalized Morse type of interaction between atoms [36]. As per our knowledge, Milstein et al [35] and Ciftci et al [2] have calculated theoretical strength of Al and found 11.1 GPa and 3.138GPa respectively by using EAM which are approximately same order in magnitude as our results.

Table 2 Strength of Al 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	2	1/5	8.5702	38.35	1.9082	-34.486
2	15	1/5	4.6863	9.216	2.55014	-38.657
6	15	1/5	4.72605	10.365	2.4654	-38.06
2	2	1/30	8.7593	46.22	1.7508	-35.5415

V. CONCLUSION

Due to presence of dislocation and imperfection in the experimental specimen, experimental results (2.254GPa) of Gane [37] are not close with our calculated results. Our results are same order in magnitude of results of other workers. It is very interesting that second phase during compression is absent which is found when we used Morse type of interaction between atoms.

VI. REFERENCES

[1] J. Cai, Phys. Status Solida B Vol.203, pp. 345, 1997.
[2] Y. Özteken Ciftci and K. Colakogeu Acta Physica Polanica A Vol.100, pp.539, 2001.
[3] J. M. Zhang, Y. Yang, K. W. Xu, V. Ji, Canadian Journal of Physics Vol.86, pp.935, 2008.
[4] J. M. Zhang, Y. Yang, K. W. Xu, V. Ji, Compt. Mater. Sci. Vol.43, pp.917, 2008.
[5] J. M. Zhang, Z. L. Lin, Y.Zhang, V. Ji, Pramana J. of Phys. Vol.742, pp.261, 2010.
[6] M.Cerny, J.Pokluda Journal of Alloys and Compound Vol.378, pp.159, 2004.
[7] D. M. Clatterbuck, D. C. Chrzan and Jr. J. W. Morris Scrip. Mater. Vol.49, pp.1007, 2003.
[8] D. M. Clatterbuck, D. C. Chrzan and Jr. J. W. Morris Phil. Mag. Lett. Vol.82, pp.141, 2002.
[9] M. Friak, M. Šob and V. Vitek Phil. Mag. Vol.83, pp.3529, 2003.
[10] M. Černy, J. Pokluda, M. Šob, M. Friak and P. Šandera Phys. Rev. B Vol.67, pp/035116, 2003.
[11] M. Černy, P. Šandera and J. Pokluda Czech. J. Phys. Vol.49, pp.1495, 1999.
[12] W. Luo, D. Roundy, M. L. Cohen and Jr. J. W. Morris Phys. Rev. B Vol.66, pp.094110, 2002.

[13] F. Milstein, J. Zhao and D. Maroudas Phys. Rev. B Vol.70, pp.184102, 2004.
[14] F. Milstein, J. Zhao, S. Chantasiriwan and D. Maroudas Appl. Phys. Letter Vol.87, pp.251919, 2005.
[15] M. A. Tschopp and D. L. McDowell Appl. Phys. Lett. Vol.90, pp.121916, 2007.
[16] M. A. Tschopp and D. L. McDowell J. Mech. Phys.Solids Vol.56, pp.1806, 2008.
[17] Vikram Singh, Gitam Singh, Research and Review: Jour. Of Phys. Vol.5 issue.3 pp.28, 2016.
[18] M. Cerny Material Science and Engineering: A Vol.4621, pp.432, 2007.
[19] M. Cerny, P. Sastak, J. Pokluda, So Phys. Rev. B Vol.87, pp.014117, 2013.
[20] P. Rehak, M. Cerney Engineering Materials Vol.592-593, pp.547, 2014.
[21] P. Rehak, M. Cerney Modelling and simul. In Mater. Sci. and Eng. Vol.23, 2015.
[22] M.Cerny, J.Pokluda Journal of Alloys and Compound Vol.378, pp.159, 2004.
[23] M. Černy, J. Pokluda, M. Šob, M. Friak, and P. Šandera Phy. Rev. B Vol.67, pp.035116, 2003.
[24] M. Černy, P. Šandera, and J. Pokluda Czech. J. Phys. Vol.49, pp.1495, 1999.
[25] D. T. Ho, S. D. Park, S.Y. Kwon, T. S. Han, S. Y. Kim Euro Physics Letters pp.111, 2015.
[26] Vikram Singh IJSER Vol.4, issue.10, pp.117, 2016.
[27] S. Ogata, Y. Umeno, M. Kohyama Modelling and Simul.in Scie. And Eng. Vol.17, 2009.
[28] Yu Zou, Jeffrey M. Wheeler, Huan Ma, Philipp Okle, and Ralph Spolenak. Phys. Nano Lett, January 2017.
[29] Duc Tam Ho,Soon Kim, Soon-Yong Kwon,and Sung Youb Kim.Mechanics materials .Vol.141, pp.103241, 2020.
[30] Bo Yang, Xianghe Peng , Henggo Xiang, Deqiang Yin, Cheng Huang, Sha Sun, Tao Fu .J.alloys and compounds, Vol. 739, pp.431-438, 2018.
[31] M.I. Baskes phys. Rev. B Vol.46, pp.2727, 1992.
[32] A.F. Voter Intermetallic Compounds, Vol.1 pp.778, 1994 (New york: Wiley).
[33] S. Chantasiriwan and F. Milstein phys. Rev. B Vol.48, pp.14080, 1996.
[34] S. Chantasiriwan and F. Milstein phys. Rev. B Vol.58, pp.5996, 1998.
[35] F. Milstein and S. Chantasiriwan phys. Rev. B Vol.58, pp.6006, 1998.
[36] Vikram Singh Deliberative Research Vol.17, issue.2, pp.1, 2013.
[37] N. Gane Proc. Soc. A Vol.317, pp.367, 1970.

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