First-principles Calculations of Twin-boundary and Stacking-fault Energies in Magnesium

Y. Wang, L. -Q. Chen, and Z. -K. Liu

Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802

S. N. Mathaudhu

Materials and Manufacturing Sciences Division, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005-5069, USA

The interfacial energies of twin boundaries and stacking faults in metal magnesium have been calculated using first-principles supercell approach. Four types of twin boundaries and two types of stacking faults are investigated, namely, those due to the $(10\bar{1}1)$ mirror reflection, the $(10\bar{1}1)$ mirror glide, the $(10\bar{1}2)$ mirror reflection, the $(10\bar{1}2)$ mirror glide, the I1 stacking fault, and I2 stacking fault. The effects of supercell size on the calculated interfacial energies are examined. The calculated interfacial energies are 85.5, 81.0, 118.1, 120.0, 8.1, and 21.8 mJ/m^2, respectively, for the six types of atomic configurations.

Keywords: magnesium; interfaces; twinning; first-principle calculation

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
JAN 2010		**00-00-2010 to 00-00-2010**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
First-principles Calculations of Twin-boundary and Stacking-fault Energies in Magnesium	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **U.S. Army Research Laboratory,Materials and Manufacturing Sciences Division,Aberdeen Proving Ground,MD,21005-5069**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**Same as Report (SAR)**	**13**	

Magnesium alloys are increasingly being used in a wide range of applications due to their light weight and high strength. One of the current research frontiers on Mg alloys is to understand, estimate, and improve their low plastic formability to operate under increasingly demanding conditions. At the atomic scale, the plastic formability is closely related to the ease of the formation of planar defects along the close packed planes, namely, twin and stacking faults [1-5]. Experimentally, direct measurements of interfacial energies require very delicate techniques and the results often show large uncertainties. For instance, the measured stacking fault energies [6-8] (and references therein) for magnesium are scattered in the range of 50 – 280 mJ/m^2. Alternatively, the steady improvement in both computer power and the efficiency of computational methods in the past few years has enabled the calculation of defect energetics at reasonable computational cost. [9] For the case of metal magnesium, existing first-principles results are scattered among specific types of twin-boundary, stacking-fault, approximation to exchange-correlation energy, and supercell size. [10-14] The main purpose of this paper is report the calculation of interfacial energies of twinning and stacking faults in magnesium from a unified theoretical framework. In particular, we report our calculated results for the $(10\bar{1}1)$ mirror reflection, the $(10\bar{1}1)$ mirror glide, the $(10\bar{1}2)$ mirror reflection, and the $(10\bar{1}2)$ mirror glide twin-boundaries together with the I1 fault and I2 stacking-faults. The effect of supercell size on the calculated interfacial energies will be discussed.

Interface supercell: Since we employ first-principles approach with periodic boundary conditions, the interfaces due to twinning and stacking faults are modeled using a supercell. In fact, the crystallographic theory of twinning [2] is rather complicated for a hexagonal close packed (hcp) metal. For the special cases of $(10\bar{1}1)$ and $(10\bar{1}2)$ twins, following Morris et al. [11], the supercells are built by first transforming the hcp structure into the orthogonal structure

(see Fig. 1) by which both the $(10\bar{1}1)$ and $(10\bar{1}2)$ planes can be seen more clearly. Secondly, the ***a*** lattice vector of the supercell is taken as that parallel to paper surface and within the $(10\bar{1}1)$ or $(10\bar{1}2)$ plane and the ***b*** lattice vector of the supercell is taken as that vertical to paper surface and within the $(10\bar{1}1)$ or $(10\bar{1}2)$ plane. Furthermore, the ***c*** lattice vector of the supercell is derived in the direction perpendicular to both ***a*** and ***b***. Then, cut away the atoms that above the interfacial plane that pass through ***a*** and ***b***, followed by making a mirror reflection with respect to the interfacial plane that pass through ***a*** and ***b***. The last step is to shift the atoms that are nearest to the interfacial plane to the interfacial plane for the mirror reflection twin or to shift the reflected atoms by ***b*** /2 for the mirror glide twin. The examples of the built supercells for the $(10\bar{1}1)$ and $(10\bar{1}2)$ twins are illustrated in Fig.2 and Fig. 3, respectively. The supercells for the I1 and I2 stacking faults are relatively easier to build. Take the case of 32-atom supercell (16-layer) as an example, they are just the ABABABABCBCBCBCB and ABABABABCACACACB arrangements, respectively, for the I1 and I2 stacking faults. [12] Note that by supercell approach, each supercell contains two interfaces. The effect of supercell sizes on the calculated interfacial energies is studied. The built supercells with different sizes are listed in Table 1.

Computational settings: To calculate the 0 K energies, we employed the Vanderbilt ultrasoft pseudopotential [15] within the generalized gradient approximation (GGA) [16] to the exchange-correlation energy as implemented in the VASP package. [17, 18] The plane wave energy cutoff is 132.7 eV which is an automatic value when setting the key "Prec=High" in VASP. The calculation of interfacial energy involves finding the difference between two total energies. We have therefore adopted very dense *k* points (See Table 1) and the Gamma centered scheme is used. We extracted the interfacial energy, ζ, by

$$\zeta = (E_{Supercell} - E_{hcp})/2A,$$

noting that $E_{Supercell}$ is total energy of the supercell, E_{hcp} is total energy of hcp Mg scaled to the supercell size, and A is interfacial area which is scalar value of the cross product of lattice vector $\boldsymbol{a}$ and $\boldsymbol{b}$. We note that in the above procedure of extracting the interfacial energy, the elastic energy resulted from the formation of interface has not been considered separately. This is a reasonable approximation for the twin-boundary in hcp Mg, as it will be seen that the calculated interfacial energies are just weakly dependent on the supercell size (See Table 1).

Results and discussions: The calculated interfacial energies are summarized in Table 1, together with and the measured stacking fault energies [6-8] and those previously calculated within different approaches. [4, 10-14] For the twin-boundaries, it is observed from our calculations that the effects of the gliding of the interfacial crystal planes on the interfacial energy are minor, and the interfacial energies of the twin-boundary are one magnitude larger than those of stacking-faults. It is further seen the effects of the supercell size on the calculated interfacial energies. For the twin-boundary, increasing the supercell size up to 80 atoms can only decrease the interfacial energy by less than 5%. However, the calculated interfacial energies for stacking-faults show strong dependence on the adopted supercell size, as it is seen from Table 1 (I1 and I2) that the calculated interfacial energies are reduced by 50% when the supercell size is increased from 8 to 32. This is because that the interfacial energies for the I1 and I2 stacking-faults are small number whose calculations have reached the accuracy limit of the current first-principles method.

We assume that the larger the supercell sizes are the more accurate of the calculated interfacial energies are. For the six largest supercells of the six types of defects, our calculated interfacial energies are 85.5, 81.0, 118.1, 120.0, 8.1, and 21.8 mJ/m^2, respectively, for the $(10\bar{1}1)$ mirror reflection, the $(10\bar{1}1)$ mirror glide, the $(10\bar{1}2)$ mirror reflection, the $(10\bar{1}2)$ mirror glide, the I1 stacking fault, and I2 stacking fault. In overall, these numbers are in good agreements with the reported results from the previous publications. Yoo et al. [14] calculated the $(10\bar{1}1)$ and $(10\bar{1}2)$ mirror reflection twins employing the *ab initio* method (no information was given on the employed potential and the approximation to the exchange-correlation energy by Yoo et al.), and reported the calculated interfacial energy values of 70 and 114 mJ/m^2, respectively; Morris et al. employed the same *ab initio* method (the same group of Yoo et al. mentioned above) to calculate the $(10\bar{1}2)$ mirror reflection and the $(10\bar{1}2)$ mirror glide twins using 20-atom supercells and reported the same interfacial energy of 114 mJ/m^2 for both the $(10\bar{1}2)$ mirror reflection and the $(10\bar{1}2)$ mirror glide twins. The calculated interfacial energies of the I1 and I2 stacking faults by Smith et al. [12] were, respectively, 9 and 18 mJ/m^2 using the 24-atom supercells (12 layers of Mg) and the ABINIT package [19] within GGA. The calculated interfacial energies of the I1 and I2 stacking faults by Chetty and Weinert [10] were, respectively, 10 and 22 mJ/m^2 using the 24-atom supercells (12 layers of Mg) within the local density approximation (LDA) [20]. The calculated interfacial energies of I2 stacking fault by Uesugi et al. [13] was 16 mJ/m^2 using CASTEP package [21] within GGA. Other results for stacking-fault energies are from the embedded atom method (EAM) by Hu et al. [4] who reported the interfacial energies are 4, and 8 mJ/m^2, respectively, for the I1and I2 stacking faults, respectively.

In summary, the interfacial energies for four types of twin boundaries and two types of stacking faults observed in metal magnesium have been obtained through first-principles

calculations. It therefore offers a unified picture of the interfacial energies for these lattice mismatches within the same theoretical framework. The calculated values can also serve as the input for the future simulation of the growth process of these planar defects or the estimation of the effects of these lattice mismatches on the mechanical properties of magnesium alloys.

Acknowledgement

The financial support from U.S. Army Research Laboratory under contract W911NF-08-2-0064 is especially acknowledged. This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Calculations were also conducted at the LION clusters at the Pennsylvania State University (supported in part by National Science Foundation Grants Nos. DMR-9983532, DMR-0122638, and DMR-0205232, and in part by the Materials Simulation Center and the Graduate Education and Research Services at the Pennsylvania State University). Additional funding from the National Science Foundation through grant DMR-0510180 is gratefully acknowledged. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the U.S. Army Research Laboratory or the U.S. Government. The U.S. Government is authorized to reproduce and distributed reprints for Government purposes not withstanding any copyright notation hereon.

[1] Serra A, Bacon DJ, Pond RC. Acta Metall 1988;36:3183.

[2] Christian JW, Mahajan S. Prog Mater Sci 1995;39:1.

[3] deDiego N, Bacon DJ. Model Simul Mater Sci Eng 1995;3:797.

[4] Hu WY, Zhang BW, Huang BY, Gao F, Bacon DJ. J Phys-Condes Matter 2001;13:1193.

[5] Capolungo L, Beyerlein IJ. Phys Rev B 2008;78:024117.

[6] Sastry DH, Prasad YVR, Vasu KI. Scripta Mater 1969;3:927.

[7] Couret A, Caillard D. Acta Metall 1985;33:1455.

[8] Fleischer RL. Scripta Mater 1986;20:223.

[9] Liu ZK. J Phase Equilib Diffus 2009;30:517.

[10] Chetty N, Weinert M. Phys Rev B 1997;56:10844.

[11] Morris JR, Ye YY, Yoo MH. Philos Mag 2005;85:233.

[12] Smith AE. Surf Sci 2007;601:5762.

[13] Uesugi T, Kohyama M, Kohzu M, Higashi K. Mater Sci Forum 2003;419-4:225.

[14] Yoo MH, Morris JR, Ho KM, Agnew SR. Metall Mater Trans A-Phys Metall Mater Sci 2002;33:813.

[15] Vanderbilt D. Phys Rev B 1990;41:7892.

[16] Perdew JP, Chevary JA, Vosko SH, Jackson KA, Pederson MR, Singh DJ, Fiolhais C. Phys Rev B 1992;46:6671.

[17] Kresse G, Furthmuller J. Phys Rev B 1996;54:11169.

[18] Kresse G, Joubert D. Phys Rev B 1999;59:1758.

[19] Gonze X, Rignanese GM, Verstraete M, Beuken JM, Pouillon Y, Caracas R, Jollet F, Torrent M, Zerah G, Mikami M, Ghosez P, Veithen M, Raty JY, Olevanov V, Bruneval F, Reining L, Godby R, Onida G, Hamann DR, Allan DC. Z Kristall 2005;220:558.

[20] Ceperley DM, Alder BJ. Phys Rev Lett 1980;45:566.

[21] Payne MC, Teter MP, Allan DC, Arias TA, Joannopoulos JD. Rev Mod Phys 1992;64:1045.

Figure 1 (color online). The $(10\bar{1}1)$ and $(10\bar{1}2)$ planes in hcp metals. The heavy (blue) and light (yellow) balls are used to represent the A and B atomic layers in *c* direction conventionally used for the hcp structure. The grey box shows the orthogonal cell mapped from the hcp cell.

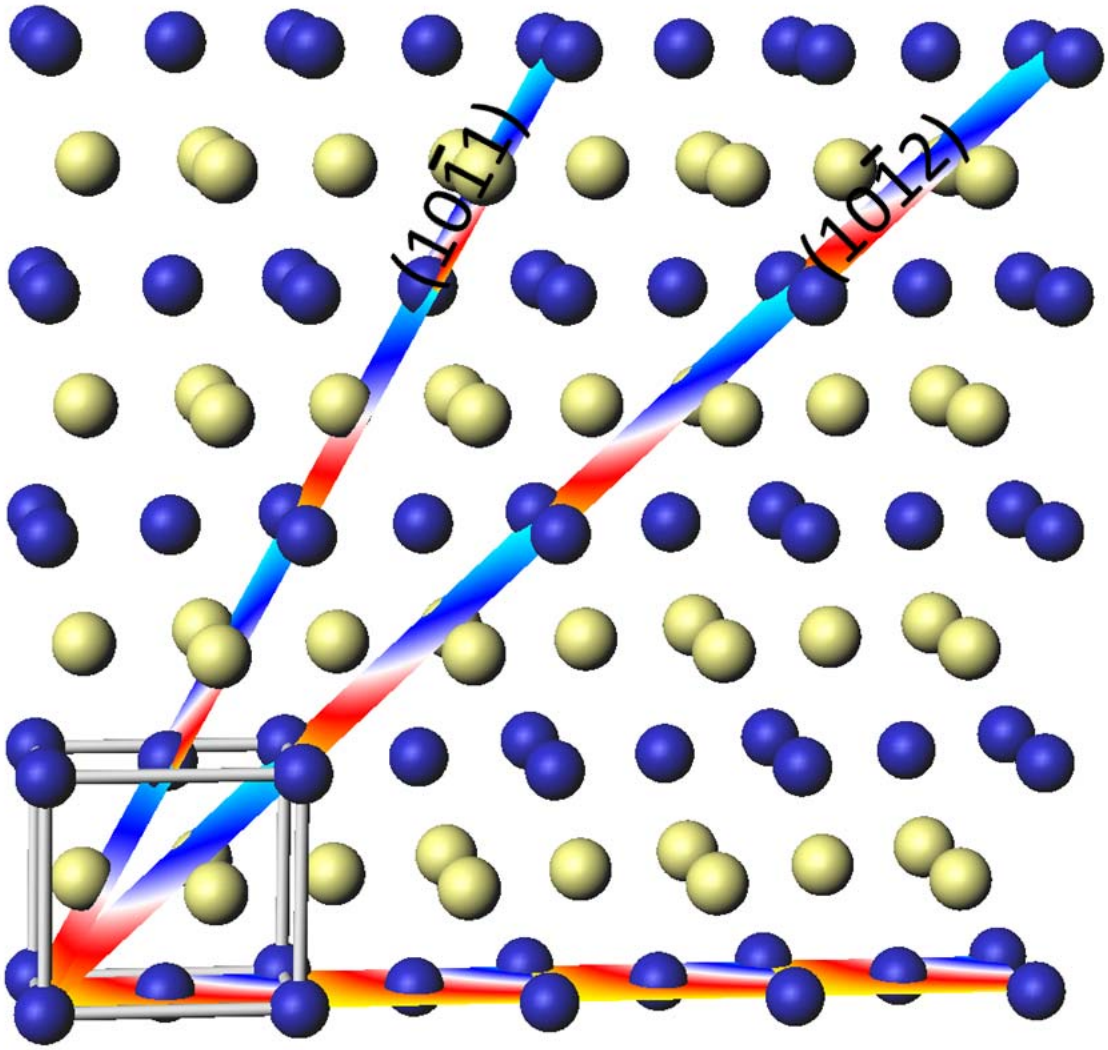

Figure 2 (color online). Structures of $(10\bar{1}2)$ mirror reflection twin-boundary (left panel) and $(10\bar{1}2)$ mirror glide twin-boundary (right panel). See also Fig. 1 for meanings of the balls.

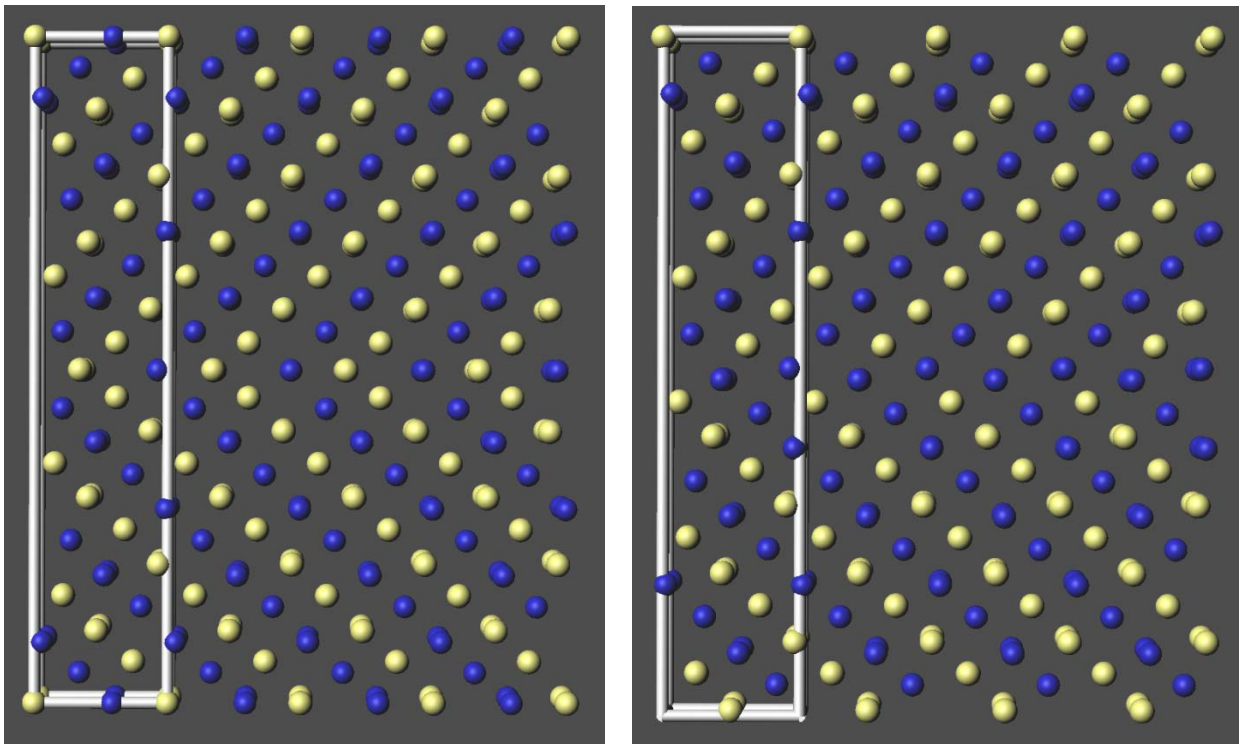

Figure 3 (color online). Structures of $(10\bar{1}1)$ mirror reflection twin-boundary (left panel) and $(10\bar{1}1)$ mirror glide twin-boundary (right panel). See also Fig. 1 for meanings of the balls.

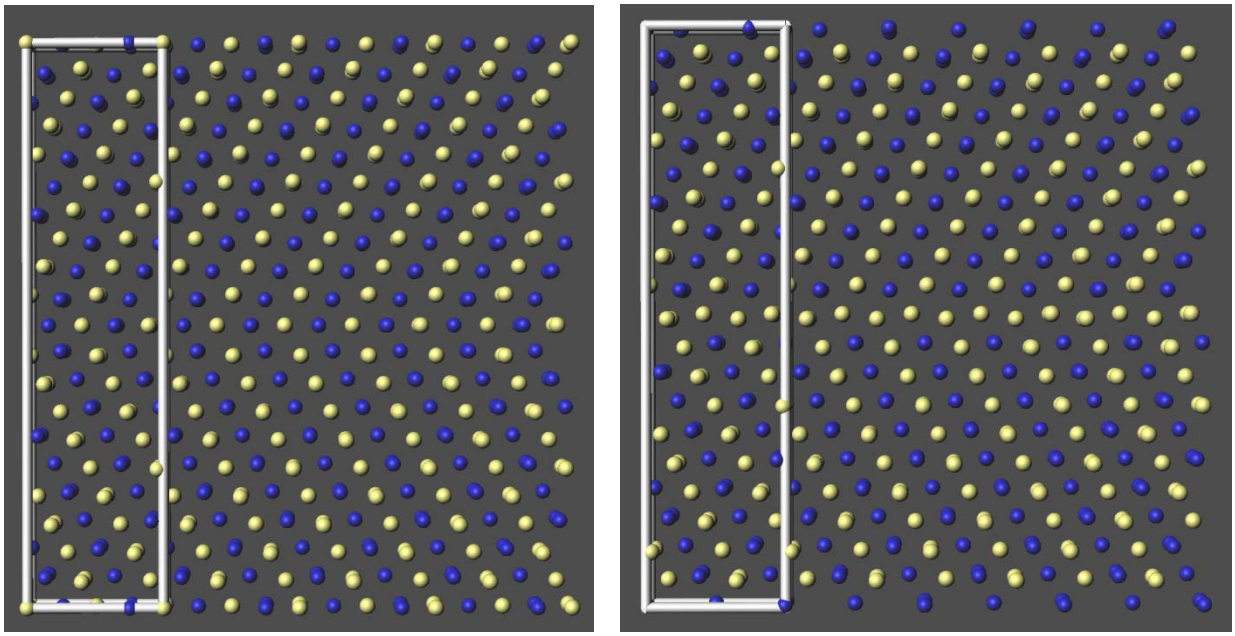

Table 1. Computational settings and interfacial energies. For the I1 and I2 stacking faults, the reported stacking fault energies in the literatures [6-8, 10, 12, 13] have been divided by a factor of two since I1 and I2 contain two interfaces [12].

	k-mesh	Supercell size	Interfacial energy (mJ/m^2)		
			This work	Previous Calculation	Measurements
hcp Mg	25×25×15	2	0.		
$(10\bar{1}1)$	7×25×4	40	84.2	70[a]	
	9×31×3	80	85.5		
$(10\bar{1}1)$g	7×25×4	40	84.2		
	9×31×3	80	81.0		
$(10\bar{1}2)$	17×39×7	20	122.3		
	11×25×3	40	118.8	114[b];114[a]	
	13×31×2	80	118.1		
$(10\bar{1}2)$g	17×39×7	20	125.3		
	11×25×3	40	120.8	114[b]	
	13×31×2	80	120.0		
I1	25×25×12	8	17.8		
	25×25×9	16	13.1	9[c]; 10[d]; 4[f]	<25[g]; 39[h]; >45[i]; 51~140[j]
	25×25×6	32	8.1		
I2	25×25×12	8	38.3	18[c]; 22[d]; 16[e]; 8[f]	
	25×25×9	16	27.7		

	25×25×6	32	21.8		

a. Yoo et al. [14], *ab initio* calculation (See the text).

b. Morris et al. [11], *ab initio* calculation (See the text).

c. Smith, [12] ABINIT 24-atom supercell within GGA.

d. Chetty and Weinert, [10] LDA.

e. Uesugi et al., GGA [13].

f. Hu et al. [4], EAM.

g. Court and Caillard. [7]

h. Sastry et al. [6]

i. Fleischer. [8]

j. Quoted by Fleischer. [8] (See references therein).