

FIRST PRINCIPLES CALCULATIONS OF STACKING FAULTS FOR TITANIUM

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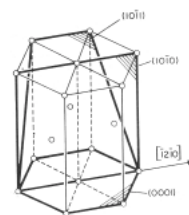
For titanium, there is considerable interest in the deformation mechanism and comparison of slip on different crystallographic planes. For hcp metals stacking faults are observed on basal, prismatic or pyramidal planes. The preponderance of particular plane observed faults for different metals has been ascribed to different c/a ratios, but this simplistic picture frequently does not fit experimental observations. In order to gain insight into some of these effects, this work presents results of a series of first principle electronic calculations using the ABINIT package [1].

Calculations have previously been performed by Smith [2] on the lowest energy stacking fault and pseudo twin structures for Mg using first principle GGA calculations. However, Ti has a complex phase diagram with a multiplicity of low energy phases other than hcp [3]. Previous work has been carried out using GGA potentials by Uesugi et al [4] in determination of the generalised stacking fault energy.

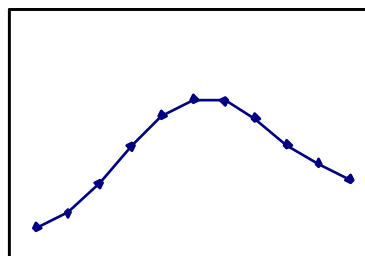
System	Atoms	Supercell	Faults	Mg Energy (meV) GGA	Ti Energy (meV) PAW
hcp	12	ABABABABAB	0	0	
fcc	12	ABCABCA BCABC		13	54
I ₁	12	ABABABCBCBCB	2	47	
I ₂	12	ABABABCACACB	2	150 (75)	
E	13	ABABABCABABAB	1	32	
T ₂	12	ABABABC BABAB	1	22	

Calculations were carried out to determine bulk properties and in particular values for cohesive energy and surface energy.

Bulk properties	Mg GGA	Mg Expt	Ti GGA PAW	Ti Expt.
$a(\text{\AA})$	3.18	3.21	2.94	2.95
c/a	1.627	1.624	1.584	1.586
cohesive energy (eV)	1.51	1.51	6.48 (5.17)	4.85
surface energy (eV)	0.30	0.28		
work function (eV)	3.72	3.84		4.33



Slip directions in hcp



Generalised stacking fault energy along basal plane

Stacking fault energies (mJ/m ²)	Mg GGA	Mg Experiment	Ti GGA	Ti Experiment
Basal	36	<50; 78	320	300
Prismatic	265			
Pyramidal	344			

The small differences in energy values from previous calculations can be ascribed to choice of density functional theory approximation, increased distance between stacking faults in periodic cell and different energy minimisation relaxation algorithms. Ti presents a particular challenge in terms of potential construction compared with Mg, presumably because of its d electrons.

References

- [1] X. Gonze et al., Comput. Mat. Sci., 25, 2002, 478-492. (The ABINIT code is a common project of the Université Catholique de Louvain, Corning Incorporated, and other contributors. See <http://www.abinit.org>.)
- [2] A.E. Smith, Surface Science, 601, 2007, 5762.
- [3] R.G. Hennig, T.J. Lenosky, D.R. Trinkle, S.P. Rudin and J.W. Wilkins, Phys. Rev. B, 78, 2008, 054121.
- [4] T. Uesugi, M. Kohyama, M. Kohzu and K. Higashi, Mat. Sci. Forum, 419-422, 2003, 225-230.