Stacking-fault energies for Cu, Ag, and Au from density-functional theory

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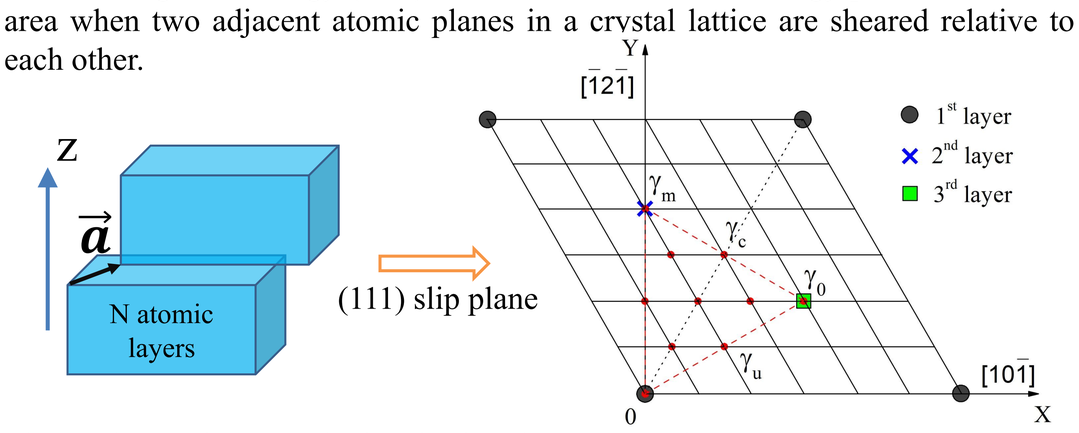
1. Motivation

The plastic deformation of fcc crystals are strongly determined by the 1/2<110> dislocation, and its geometric structure can be traced back to the {111} γ-surface. A precise knowledge of selected points on this surface is, hence, of essential importance. Unfortunately, experimental and theoretical results are varying over a wide range, which is related to the fact that the energetic differences can be very small, it is in the meV/atom range. Using density-functional theory (DFT) we calculate the stacking-fault energies for the {111} surface of Cu, Ag, and Au. The computational efficiency and accuracy of several different approaches are investigated. Strong emphasis is laid on the convergence with respect to the k point sampling. The influence of slab thickness and relaxation of unit-cell parameters and atomic positions is also examined. With our procedures, the stacking-fault energies are obtained with very high precision.

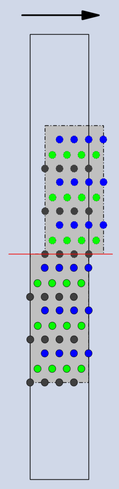
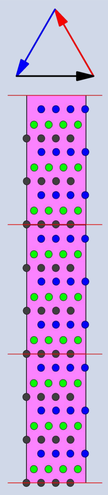
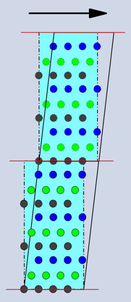
2. Method

The stacking-fault energy (SFE) is defined as the excess energy per unit interface area when two adjacent atomic planes in a crystal lattice are sheared relative to each other.

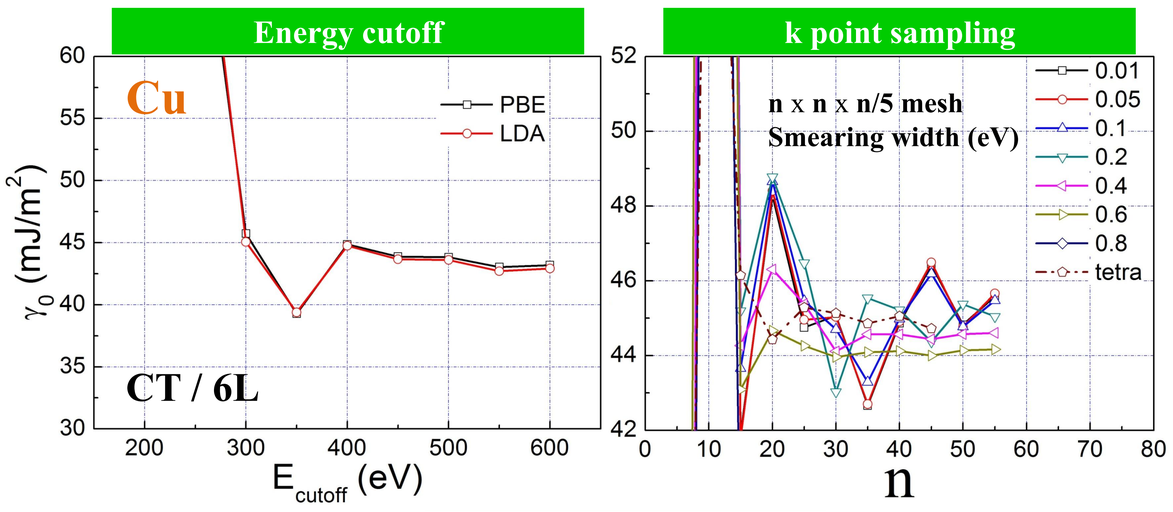


The total-energies are calculated using the VASP code.

3. Comparison of models

Model	Axial-Next-Nearest-Neighbor-Ising Model (ANNNI)	Slab-Shift Model (SS)	Displacement-Shift-Complete Model (DSC)	Cell-Tilt Model (CT)
Structure	fcc ABCABC… hcp ABABAB… dhcp ABACAB… thcp ABCACB…			
Formula	$\gamma_0^{(1)} = \frac{2E_{hcp} - 2E_{fcc}}{A}$ $\gamma_0^{(2)} = \frac{2E_{dhcp} + E_{hcp} - 3E_{fcc}}{A}$	$\gamma = \frac{E_{shift} - E_0}{A}$	$\gamma = \frac{E_{shift} - E_0}{3A}$	$\gamma = \frac{E_{tilt} - E_0}{A}$
No. of layers	≤ 6	2N	3N	N
Vacuum	×	✓	×	×
Relaxation	×	✓	✓	✓
Full γ–surface	×	✓	✓	✓

4. Convergence



Differences between models

System	Relax z-force	ANNNI $\gamma_0^{(1)}$	ANNNI $\gamma_0^{(2)}$	SS γ_0 (12L)	SS γ_0 (18L)	CT γ_0 (6L)	CT γ_0 (9L)
Cu	×	45	46	42	42	45	46
	✓	-	-	41	42	44	45

CT model: number of layers and relaxation of stress

System	Relax	Layers (L)	γ_0	γ_u	γ_c	γ_m
Cu	z-force	6	44	169	537	936
		9	45	171	526	902
		12	42	169	520	880
		18	45	169	512	865
	z-stress	9	48	170	503	832

5. Bulk properties

System	Type	a_0 (Å)	B (GPa)	C_{11} (GPa)	C_{12} (GPa)	C′ (GPa)	C_{44} (GPa)
Cu	PBE	3.636	139.06	174.78	121.19	26.08	78.93
	LDA	3.523	187.34	231.60	165.21	33.19	99.03
	Exp.[1-3]	**3.615**	**142.03**	**176.20**	**124.94**	**25.63**	**81.77**
Ag	PBE	4.164	89.42	109.11	79.57	14.77	40.99
	LDA	4.015	138.20	165.89	124.35	20.77	58.90
	Exp.[1-3]	**4.086**	**108.72**	**131.49**	**97.33**	**17.08**	**51.09**
Au	PBE	4.175	136.76	151.56	129.37	11.10	26.47
	LDA	4.062	192.62	211.55	183.15	14.20	37.23
	Exp.[1-3]	**4.079**	**180.32**	**201.63**	**169.67**	**15.98**	**45.44**

6. Stacking-fault energies (mJ/m^2)

System	Type	ANNNI γ_0	CT / 9L γ_0	CT / 9L γ_u	CT / 9L γ_c	CT / 9L γ_m	Exp.[4] γ_0
Cu	PBE	46	45 (48)	171 (170)	526 (503)	902 (832)	**45**
	LDA	56	52 (52)	206 (202)	641 (610)	1099 (1017)	
Ag	PBE	16	16 (16)	97 (95)	307 (289)	507 (456)	**16**
	LDA	29	29 (28)	134 (131)	422 (396)	693 (624)	
Au	PBE	30	28 (28)	78 (75)	257 (230)	394 (326)	**32**
	LDA	38	34 (34)	101 (97)	344 (309)	530 (443)	

* Results from stress relaxation are listed in brackets.

7. Conclusions

Performing well-converged calculations, consistent $\gamma_0$values between the ANNNI model and the CT model are revealed, indicating a reliable determination of SFEs from DFT. Relaxing the z components of force and stress has small influence on γ_0 and γ_u, but leads to a much quicker convergence of γ_c and γ_m with respect to the number of atomic layers used in the most efficient method, which is the CT model. The SFEs calculated with this procedure are of high precision, and the values agree better with the most trustable experimental results than previous DFT calculations.

8. References

[1] W. B. Pearson, *Handbook of Lattice Spacing and Structure of Metals and Alloys*, Pergamon, Oxford, 1967.

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