

Lawrence Berkeley National Laboratory

Recent Work

Title

PSEUDOPOTENTIAL CALCULATION OF THE STACKING FAULT ENERGY IN DIAMOND, GERMANIUM, AND GREY TIN

Permalink

<https://escholarship.org/uc/item/9jm5t20x>

Authors

Chen, L.J.
Falicov, L.M.

Publication Date

1974-03-01

Submitted to the Philosophical Magazine

LBL-2594
Preprint *c.j.*

PSEUDOPOTENTIAL CALCULATION OF THE STACKING
FAULT ENERGY IN DIAMOND, GERMANIUM, AND GREY TIN

L. J. Chen and L. M. Falicov

RECEIVED
LAWRENCE
RADIATION LABORATORY

March 1974

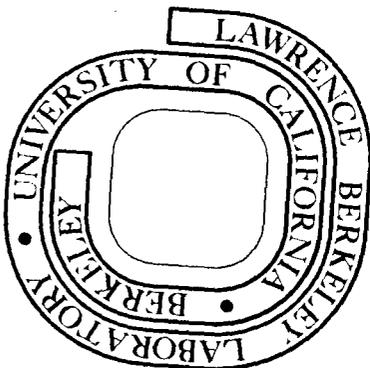
APR 1 1974

LIBRARY AND
DOCUMENTS SECTION

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48

TWO-WEEK LOAN COPY

This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 5545



25

LBL-2594
c.j.

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

PSEUDOPOTENTIAL CALCULATION OF THE STACKING
FAULT ENERGY IN DIAMOND, GERMANIUM, AND GREY TIN.

L.J. CHEN

Department of Physics, University of California, and
Inorganic Materials Research Division, Lawrence Berkeley Laboratory,
Berkeley, California, 94720, USA

and

L. M. FALICOV*

Department of Physics, University of California
Berkeley, California, 94720, USA

* Work supported in part by the National Science Foundation
through Grant NSF-GH 34438.

ABSTRACT

The intrinsic stacking fault energy of diamond, germanium and grey tin have been calculated by the pseudopotential method to a second order perturbation approximation. The calculated value for germanium, 26 erg/cm^2 , falls within 50% of the experimental value determined by the weak beam technique in electron microscopy. The value for diamond, questionable because of possible poor convergence of the method, is very large, 1860 erg/cm^2 . Grey tin exhibits a small value, 3 erg/cm^2 , which could in principle be easily measured experimentally.

In a previous paper (I) (Chen and Falicov, 1974), we reported the result of a pseudopotential (PP) calculation of the intrinsic stacking fault energy (SFE) of silicon. The calculated value, 55 erg/cm^2 , was in remarkably good agreement with experimental data and prompted us to calculate SFE's of the other diamond structure elements - diamond, germanium, and grey tin - with the same method.

The formulation follows exactly that of I. The parameter used for the three materials are listed in Table 1; all quantities are in atomic Rydberg unit.

The experimental (fitted) values of the screened PP form factor as given by Au-Yang and Cohen (1969) are given in the Table 2.

As in the calculation for silicon, we use two interpolation formulae: either that of Falicov and Golin (1965)

$$v_b(q) = (Aq^2 + B) [C \exp(Dq^2) + 1]^{-1} \quad (1)$$

or a quadratic form

$$v_b(q) = Eq^2 + Fq + G \quad (2)$$

The parameters in (1) and/or (2) are chosen so as to obtain a continuous function of q . The fitted values follow.

(1) Diamond:

We use formula (1) for the whole needed range

$q > q_c = 1.320$ with

$$A = 0.2678$$

$$B = -1.514$$

$$C = 4.579 \times 10^{-7}$$

$$D = 1.716$$

(2) Germanium:

We use (1) for $q \geq 1.469$ with

$$A = 0.0896 \qquad B = -0.2366$$

$$C = 4.629 \times 10^{-6} \qquad D = 2.988$$

and (2) for $1.469 \geq q \geq q_c = 0.832$ with

$$E = -1.075 \qquad F = 3.067 \qquad G = -2.229.$$

(3) Grey tin:

We use (1) for $q \geq 1.287$ with

$$A = 0.089 \qquad B = -0.1594$$

$$C = 1.874 \times 10^{-3} \qquad D = 2.825$$

and (2) for $1.287 \geq q \geq q_c = 0.728$ with

$$E = 0.8404 \qquad F = -1.304 \qquad G = 0.2757$$

The structure factors and method of calculation are exactly the same as those in I. The results are listed in Table 3.

As far as the authors are aware, only the experimental data for the SFE of Ge are available. Häussermann and Schaumburg (1973) observed the separation of two partials of extended 60° and edge dislocations to be $54 \pm 11 \overset{\circ}{\text{Å}}$ by means of the weak beam method in electron microscopy (Cockayne et al 1969).

From the dislocation theory of crystals, edge dislocations

may dissociate into two partial dislocations with larger separation. Since Häussermann and Schaumburg do not give detailed account of specific values of separation for specific type of dislocation, and since edge dislocations are in general separated into partials with larger distances than 60° ones, we take 65 \AA (the upper value they quote) as the separation between partials of an edge dislocation. In such a case with the assumption of isotropic elasticity, the SFE can be calculated to be 38 erg/cm^2 . The relation between equilibrium separation of two partial dislocations and the SFE has been taken from Read (1953), and we have used the isotropic elastic constant from the list compiled by Gshneidner (1964). For the anisotropic case, putting the anisotropic elastic constant compiled by Huntington (1958) into the equation derived by Chou and Eshelly (1962), the SFE is 45 erg/cm^2 .

It is encouraging to see that the theoretical value, although smaller than both experimental estimates, is within 30% of the smaller one and 50% of the larger one. This is a priori the type of accuracy which we would expect from a second-order PP calculation.

The calculated SFE for diamond seems to be much too large, even after taking into account the extremely strong bonding properties of the C-C links. It is, however, known that the

PP method converges rather slowly (Cohen and Heine, 1970) for elements in the second row of the periodic table, where no p-electrons exist in the core. The value in Table 3, although indicative and probably correct in order of magnitude, should not be considered an accurate one.

The theoretical value of the SFE for grey tin suggests that the extended dislocation separation for this unstable phase of Sn should be about 700\AA . This can be easily measured in principle in the electron microscope.

We have tested the sensitivity of our results to the accuracy of the interpolation formulae (1) and (2), and we have found that the values quoted in Table 3 change by a negligible 0.5% at most if a reasonable change of 20% is induced in the position of the zero of $v_b(q)$

In conclusion, we would like to point out that the general agreement obtained for Si and Ge between theory and experiment, and the sensible variation found in the changes down column IV of the periodic table strongly suggest that it will be worthwhile to extend these calculations to estimate SFE's of the III - V and II - IV zincblende structure semiconductors.

ACKNOWLEDGEMENT

The authors are grateful to Professor G. Thomas for many helpful discussions. They would like also to express their thanks to Professor J. W. Morris, Jr., for the generous consent to the use of his computing facilities. The work was done under the auspices of the U.S. Atomic Energy Commission and the National Science Foundation.

Table I

Parameters of Diamond Structure Elements

Elements	C	Ge	Sn
Cubic lattice constant a_0	6.730	10.681	12.212
Fermi wavevector k_F	1.4595	0.9196	0.8043
Smallest projection of a reciprocal lattice vector onto the fault plane G_{\perp}	1.3204	0.8320	0.7276
Density of atoms in the fault plane ω	0.0883	0.0351	0.0268

Table 2
Screened Pseudopotential Form Factors

C		Ge		Sn	
q	v(q)	q	v(q)	q	v(q)
1.62	-0.811	0.899	-0.34	0.787	-0.23
2.648	0.337	1.039	-0.203	0.909	-0.215
3.106	0.132	1.469	-0.043	1.287	-0.01
3.24	0.041	1.723	0.035	1.509	0.02
		1.8	0.05	1.575	0.02
		2.08	0.052	1.819	0.006
		2.266	0.01	>1.982	0
		>2.324	0		

Table 3
Calculated Value of SFE

Element	Stacking Fault Energy	
	atomic units	egs units
C _{diamond}	2.39×10^{-3}	1860
Ge	3.3×10^{-5}	26
Sn _{grey tin}	3.79×10^{-6}	3

REFERENCES

- AU-YANG, M.Y., and COHEN, 1969, Phys. Rev., 178, 1358.
- CHEN, L.J., and FALICOV, L.M., 1974, Phil. Mag., (in press).
- CHOU, Y.T., and ESHELLY, J.D., 1962, J. Mech. Phys. Solids,
10, 27.
- COCKAYNE, D.J.H., RAY, I.L.F., and WHELAN, M.J., 1969,
Phil. Mag., 20, 1965.
- COHEN, M.L., and HEINE, V., 1970, Solid St. Phys., 24, 37.
- FALICOV, L.M., and GOLIN, S., 1965, Phys. Rev., 137, A871.
- GSHNEIDNER, Jr., K.A., 1964, Solid St. Phys., 16, 275.
- HAUSSERMANN, F., and SCHAUMBURG, H., 1973, Phil. Mag., 27, 745.
- HUNTINGTON, H.B., 1958, Solid St. Phys., 7, 213.
- READ, W.T., 1953, Dislocations in Crystals, p. 131 (New York:
McGraw-Hill)

LEGAL NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720