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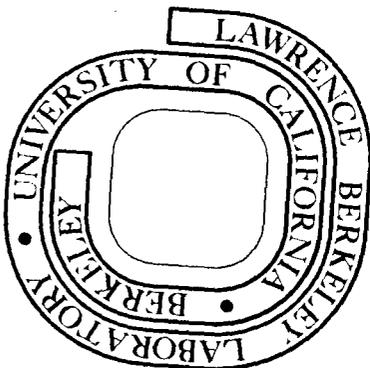
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DISCLAIMER

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

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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)

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

or a quadratic form

$$v_b(q) = Eq^2 + Fq + G \tag{2}$$

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 x 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 $54 \pm 11 \overset{\circ}{A}$ 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 $\overset{o}{A}$ (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 anistropic case, putting the anistropic

elastic constant compiled by Huntington (1958) into the equa-

tion 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 pro-

perties 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$\overset{o}{A}$. 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

Table I

Parameters of Diamond Structure Elements

Elements	C	Ge	Sn
Cubic lattice constant a_o	6.730	10.681	12.212
Fermi wave vector 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	cgs units
$C_{diamond}$	2.39×10^{-3}	1860
Ge	3.3×10^{-5}	26
$Sn_{grey\ tin}$	3.79×10^{-6}	3

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