Submitted to
Philosophical Magazine

LBL-1864
Preprint c. 1

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July 1973

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

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PSEUDOPOTENTIAL CALCULATION OF THE STACKING FAULT ENERGY IN SILICON

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

ABSTRACT

A calculation of the intrinsic stacking fault energy in silicon has been carried out to second order perturbation in the pseudopotential formalism. The calculated result is 55 erg/cm^2, which is in remarkably good agreement with the experimental value.

§INTRODUCTION

The numerical values of stacking fault energies are important parameters in the theory of plastic deformation. The experimental determination of those values has improved enormously in the last few years with the development of the weak beam technique in electron microscopy (Cockayne et al, 1969). The method has been used to determine the separation of partial dislocations, from which stacking fault energies can be obtained. It has been applied to various systems: Cu - 10% Al (Cockayne et al, 1969), silicon (Ray and Cockayne, 1970), copper and silver (Cockayne et al, 1972), gold (Jenkins, 1972), germanium (Häussermann and Schaumburg, 1973) and more recently boron-implanted silicon (Chen and Thomas, to be published).

The most important advantage of the weak beam technique is the narrowness of the image width. The image peak defines accurately the position of the partials; it is possible therefore to resolve closely spaced partial dislocations for crystal with high stacking fault energy. But the requirements for the resolution of dislocation separation of the order of 40 Å or so are so extremely stringent that it is very desirable to have a theoretical estimate of stacking fault energies on hand so as to save fruitless efforts to the experimentalist in this field.

Hodges (1967) developed a calculational method to obtain stacking fault energies in closed-packed simple metals. He used a pseudopotential (PP) formulation (Harrison 1966, Heine 1970, Cohen and Heine 1970, Heine and Weaire 1970) applied to second order in perturbation theory. His calculations, which made use of the model potentials of Heine and Abarenkov (1964), confirmed the experimental trend (large value for Al, low for Pb) but were not very accurate and even gave negative values for Pb and Zn. Hodges attributed his discrepancies to (a) the uncertainty of the PP for large momentum transfer $\vec{q}$, (b) the use of a local PP instead of a non-local angular-momentum dependent one.

The use of PP is a natural one for this kind of problem: it is conceptually simple, easy to handle and known to be accurate to about 1% in the determination of one-electron properties and say 20% in structural properties <u>whenever volume effects do not play a role</u>. Such is the case in our stacking fault problem.

From the point of view of simplicity of the numerical procedures, a local PP is undoubtedly a very desirable feature. It is known however that local PP only work well for a small number of elements on the periodic table, and usually very well only for Na, Mg, Al and Si.

We have chosen to determine the stacking fault energy in diamond-structured silicon for several reasons:

(i) The PP is very well known and has been repeatedly tested (Cohen and Heine 1970, Au-Yang and Cohen, 1969) against many experimental data.

(ii) A local PP works extremely well for silicon.

(iii) The experimental value of the stacking fault energy (Ray and Cockayne, 1970), 55 erg/cm^2 is well known and more accurate than most.

(iv). An intrinsic stacking fault in Si does not change the local tetrahedral coordination of any atom and therefore chemical-bond arguments (Phillips 1969) point out to the suitability of PP schemes and ordinary linear screening theory.

(v) The stacking fault properties can be used to supplement information on the properties of the various polytypes and amorphous forms of silicon, which are presently the subject of intensive studies (Joannopoulos and Cohen, 1973).

(vi) We would like to test a PP calculation of this sort to see whether in an open structure (e.g. the diamond structure) it works better than in a closed-packed one.

In section 2 we present the details of the calculation. Section 3 contains a brief discussion.

§2. FORMULATION OF THE PROBLEM AND CALCULATION

As discussed by Hodges (1967) and in the introduction, second order perturbation theory should give adequate results for evaluating stacking fault energies; this is primarily so because such a fault is a rearrangement of atoms at constant density. This eliminates volume dependent effects which are so sensitive to electron-electron correlations and make the Hartree (mean field) approximation a reasonable one to treat many-electron effects. In addition, since the tetrahedral coordination of each atom is preserved, the so-called bond charge (Phillips 1969) does not get appreciably

disturbed and therefore the non-linear screening properties remain unchanged throughout the calculation. Under these conditions the energy of formation of a stacking fault, neglecting correlation and exchange contributions, is given by (Hodges 1967)

$$\Delta E_{SF} = -\frac{Z^2 e^2}{(2\pi)^2} \int \frac{[\phi(q) - 1]}{q^2} \{ |S(\vec{q})|^2 - |S^0(\vec{q})|^2 \} d\vec{q} \qquad (2.1)$$

where

$$\phi(q) = -\frac{v_b^2(q)\, q^4}{(4\pi e^2)^2} \frac{1}{Z^2} \epsilon_0(q) \{\epsilon_0(q) - 1\} , \qquad (2.2)$$

$v_b(q)$ is the screened PP form factor, $\epsilon_0(q)$ is the Lindhard-Hartree dielectric function (Harrison 1966), Z is the valence of the ions (Z = 4 for silicon), $S^0(\vec{q})$ is the structure factor for the perfect lattice and $S(\vec{q})$ is the structure factor for the lattice with the stacking fault. We must now:

(a) Choose a good PP form factor $v_b(q)$ and express it in a convenient form so as to be able to integrate (2.1);

(b). Calculate the structure factors S^0 and S;

(c) Evaluate (2.1).

2.1 The PP Form Factors

The experimentally fitted values of the screened PP form factors, as given by Au-Yang and Cohen (1969) are given in table I. For our purposes, since we need $v_b(q)$ as a continuous function of q, it is necessary to use an accurate interpolation formula. We find it convenient to use (Falicov and Golin, 1965)

$$v_b(q) = (Aq^2 + B)[C \exp(Dq^2) + 1]^{-1} \tag{2.3}$$

for $q \geq 1.612$ a.u. with

$$A = 0.1449 \qquad B = -0.3767 \qquad C = 0.0061 \qquad D = 1.3568 \ . \tag{2.4}$$

For smaller values of q ($0.865 \leq q \leq 1.612$) we use a quadratic form

$$v_b(q) = -1.6545 + 2.0399\, q - 0.6288\, q^2 \ . \tag{2.5}$$

In all these formulae q is in atomic units (inverse Bohr radii) and v_b is expressed in Rydbergs. Values of v_b for $q < 0.865$ are not needed in the calculation.

2.2 The Structure Factors

We may think of a perfect silicon crystal as being made by the proper stacking of (111) type of atomic planes. Each of these planes contains a hexagonal (closed packed) arrangement of silicon atoms. The nearest neighbor separation of atoms in each of these planes is

$$a_0 = a/\sqrt{2} = (10.26/\sqrt{2})\text{a.u.} = 7.26 \text{ a.u.} \tag{2.6}$$

The two basic (period) vectors in these planes are

$$\begin{aligned} \vec{t}_1 &= a_0 \hat{y} \\ \vec{t}_2 &= a_0[0.5\, \hat{y} + (\sqrt{3}/2)\hat{z}] \ . \end{aligned} \tag{2.7}$$

There are three kinds of planes, labelled A, B and C and such that

A has an atom at $\vec{\tau}_A = 0$

B has an atom at $\vec{\tau}_B = \frac{1}{3}(\vec{t}_1 + \vec{t}_2) \equiv \vec{\tau}$

C has an atom at $\vec{\tau}_C = -\vec{\tau}$

in their respective planes. We build now the perfect lattice by following the stacking prescription:

$$\cdots AABBCCAABBCCAA\cdots$$

such that two consecutive planes of the same kind are separated by a distance (perpendicular to $\vec{t}_1$ and $\vec{t}_2$)

$$\theta_1 = a\sqrt{3}/4 = 4.44 \text{ a.u.}$$

and two consecutive planes of different kind are separated by

$$\theta_2 = a\sqrt{3}/12 = 1.48 \text{ a.u.}$$

Since the planes come always in pairs (AA), or (BB), or (CC), we can denote each pair by its corresponding primed letter, and therefore the silicon perfect crystal is given by

$$\cdots A'B'C'A'B'C'\cdots \tag{2.9}$$

each double plane being separated from its nearest neighbors by a distance

$$\theta = \theta_1 + \theta_2 = 5.92 \text{ a.u.} \quad .$$

An <u>intrinsic</u> stacking fault is now obtained by eliminating one double plane (two atomic planes), i.e.

$$\cdots A'B'C'B'C'A' \cdots \quad . \tag{2.10}$$

This is the lowest energy fault, since it preserves the tetrahedral environment of each silicon atom. It has however a small sequence

$$[B'C'B'C']$$

which corresponds to a wurtzite (rather than diamond) type structure.

We may remark now that since the diamond structure in the f.c.c. structure with a basis (two atoms per unit cell), and since the (2.9) and (2.10) sequences are identical to those discussed by Hodges (1967) for the f.c.c. intrinsic fault, our structure factors can only differ from his by a correction factor which takes the basis into account

$$S_{diamond}(\vec{q}) = [1 + \exp(-i\vec{q}\cdot\vec{\theta}_1)]S_{fcc}(\vec{q}) \tag{2.11}$$

where

$$\vec{\theta}_1 = \theta_1\hat{z} = 4.44\hat{x}\ \text{a.u.} \quad . \tag{2.12}$$

This relationship (2.11) applies both to the perfect and the stacking fault structures. We therefore obtain our structure factors easily by applying (2.11) and extracting S_{fcc} and S^0_{fcc} directly from Hodges's results.

2.3 Evaluation of the Integrals

The evaluation of (2.1) follows the standard procedure (Harrison 1966, Hodges 1967) of separating the integral into singular and non-singular parts. The singular contribution is obtained analytically and reduced to the summation of a finite series.

The non-singular part is integrated numerically using the values of $v_b(q)$ given by (2.3) and (2.5) and the analytic expression of Lindhard's dielectric function $\epsilon_0(q)$ (Harrison 1966). The results are

$$\Delta E_{SF} = W \times 7.04 \times 10^{-5} \text{ Ryd} \tag{2.13}$$

where W is the area of the stacking fault. Reduction to cgs units yields

$$\Delta\epsilon_{SF} = 55 \text{ ergs/cm}^2 \ . \tag{2.14}$$

§3 DISCUSSION

The quoted experimental values for the intrinsic stacking fault energy in silicon range from 50 erg/cm^2 (Aerts et. al, 1962) to 55 erg/cm^2 (Ray and Cockayne, 1970). The latest value is considered more accurate and reliable. Our results are in remarkably and probably fortuitously good agreement with experiment. The approximations involved in our calculation are:

(1) Those inherent in the PP formalism;

(2) Second order perturbation theory;

(3) Empirical PP form factors;

(4) Local PP approximation;

(5) Hartree approximation (no exchange and correlation corrections);

(6) Lack of inclusion of non-linear screening (influence of bond charges);

(7) Numerical and rounding off errors.

Of these we have tried to keep (7) to a reasonable value so as to ensure two significant figures of the final result; (1) is probably negligible if taken

in conjunction with (3) (Cohen and Heine 1970); (4) is very small for silicon but may be more significant for heavier or lighter semiconductors.

Since the stacking fault calculation involves no volume change, (2) is a very good approximation (Harrison 1966), and so is (5).

In the evaluation of the integral (2.1) the difference $\{|S(\vec{q})|^2 - |S^0(\vec{q})|^2\}$ vanishes for values of q smaller than $G_\perp = 0.865$ a.u. (this is the smallest non-vanishing projection of a reciprocal lattice vector onto the stacking fault plane). Therefore the dielectric function $\epsilon_0(q)$ is needed only for $q > G_\perp$, i.e. a region outside the range where the semiconducting character of the crystal and the bond charge make a sizeable difference (Phillips 1969); hence (6) should be also a good approximation.

In summary, (1)-(7) are all justifiable and the errors should be small. It is however very surprising that our agreement with experiment is so good, and this can be only fortuitous. We are nonetheless encouraged by the results and feel that similar calculations should be extended to other semiconductors to test further the validity of the theory.

ACKNOWLEDGMENT

We are grateful to Professor G. Thomas for many enlightening discussions. One of us (LJC) would like to acknowledge Professor Thomas's encouragement and guidance in getting started in this research.
This work was partially done under the U. S. Atomic Energy Commission.

Table I

Screened Pseudopotential Form Factors

q atomic units	v_b Rydbergs
0.898	-0.33
1.037	-0.215
1.467	-0.015
1.720	0.039
1.797	0.055
2.076	0.079
2.262	0.056
2.319	0.04

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