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ENERGY OF GRAIN BOUNDARIES IN SEMICONDUCTORS

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1. Introduction.- Polycrystalline semiconductors and ceramics are already widely used throughout the electronic industries for a variety of purposes: solar cells, poly-silicon thin film devices, ceramic varistors to name only a few. These commercially important devices owe their electronic properties to the presence and the character of their grain boundaries. This has motivated much of the research to investigate the microstructure, micro-chemistry and the electronic properties of the grain boundaries. However, many of the fundamental questions are still open and as a result improved materials and devices have been developed largely by empirical processes. Nonetheless it is very desirable to investigate the basic properties of single grain boundaries since that can serve as a useful background material for the device-oriented questions.

Many of the properties of grain boundaries can only be understood if their atomic- and microstructure is known [1-3]. At present, however, one can only hope to solve fundamental problems for the case of very special simple structures as they are expected for low angle and coincidence boundaries. Mainly two complementary ways of investigation can be pursued: high resolution and related electron microscopy techniques and computer calculations of the atomic structures. For semiconducting materials with its covalent bonding the latter is especially difficult since the development of the theory of the structure of defects in semiconductors is by far not completed. The most reliable results are available for point defects and surfaces in...
elemental semiconductors, however, the methods developed for these cases cannot be transferred immediately to dislocations and grain boundaries. Therefore some less sophisticated methods have been tried and applied to dislocations [4,5] and now to grain boundaries, too, as will be discussed in the following [6].

All calculations of the energy of an atomic arrangement as well as the interpretation of high resolution microscopy images can only be performed on the basis of an already approximately known atomic structure. The simplest grain boundary structures are likely to occur for coincidence orientations of the neighboring grains since that leads to periodic atomic arrangements. In such cases geometric stick and ball models can sometimes be easily obtained and for a variety of coincidence grain boundaries such atomic structures have been proposed [7,8,9]. On the basis of some of these models energy calculations have been carried out [6] and first results on [011] tilt boundaries will be presented. This type of boundary has been chosen since most of the experimental and theoretical work has been accumulated here.

2. Geometrical modeling. - Misorientations of the adjacent grains for which a periodic boundary structure occurs can be predicted by Bollmann's O-lattice theory [10]. Following this method it is convenient to introduce a coordinate system which contains the rotation axis and the plane perpendicular to it. Since all of the following calculations were performed for tilt boundaries with a [011] rotation axis we can adopt the following tetragonal unit cell to describe the diamond cubic lattice [Fig. 1].

\[ \hat{a}_1 = a[100] \quad \hat{a}_2 = \frac{a}{2}[01\overline{1}] \quad \hat{a}_3 = \frac{a}{2}[011] \]

\( a \) is the lattice constant of the conventional diamond cubic fcc unit cell to which all planes and directions will be referred unless otherwise stated [9].

Fig. 1: Projection of the diamond cubic lattice on a (011) plane. The filled and open circles are atoms at height 0 and \( a/2\sqrt{2} \), respectively.

It should be mentioned that the origin of the coordinate system does not need to be a crystal lattice point. After a rotation of one lattice with respect to another a general coincidence lattice (O-lattice) occurs for certain angles.

I we refer to the tetragonal unit cell of Fig. 1 we see that after a rotation of \( \Theta = 2 \arctan k_2/k_1\sqrt{2} \) (\( k_1, k_2 \) integer numbers) a vector \([k_1, k_2, 0]_{\text{tettr}} \) becomes coincident with \([k_1, k_2, 0]_{\text{unrot}} \) of the unrotated lattice because (01\overline{1}) is a symmetry plane of the lattice. A basis of
the 0-lattice can be derived

\[ b_1 = \frac{1}{2k_2} [k_2, 2k_1, 0]_{\text{tet}} \]

\[ b_2 = \frac{1}{2k_2} [k_1, 2k_2, 0]_{\text{tet}} \]

\[ b_3 = [001]_{\text{tet}} \]

(common integer factors have to be simplified).

In general the 0-lattice contains no crystal lattice points at all if the origin of the coordinate system has been chosen arbitrarily. In case that the origin is a lattice point the 0-lattice contains a super-lattice which consist of all crystal lattice points at coinciding positions: the coincidencesite lattice (CSL). The basis vectors are given by

\[ b_1^{\text{CSL}} = 2k_2 b_1 \]

\[ b_2^{\text{CSL}} = b_3 \]

\[ b_2^{\text{CSL}} = 2k_2 b_2 \]

The volume of the CSL unit cell is \( V_{\text{CSL}} = \Sigma a^3/2 \), where \( \Sigma = 2k_1^2 + k_2^2 \) (if \( \Sigma \) is even it has to be divided by 2) characterizes the CSL for a given rotation axis. For a fixed misorientation \( \theta \) of the two lattices, two degrees of freedom remain for the orientation of the grain boundary. Periodic grain boundary structures occur if the boundary plane is a lattice plane of the CSL. In the following only symmetric tilt boundaries are considered (unless otherwise stated) where the boundary plane is a mirror plane of the CSL and contains the [011] direction. (Relative translations of the two lattices are not considered yet). The various CSL and grain boundary orientations which have been investigated are given in table 1.

Table 1: CSL boundary orientations and energies (erg/cm²) for \( \Sigma \leq 33 \). The meaning of \( \gamma_{\text{app}}, \gamma_{\text{comp}} \) and \( \gamma_{\text{dil}} \) is explained in the text. (\( E_0 \) in ev). (*) These orientations did not yield low energy structures.

<table>
<thead>
<tr>
<th>( \Sigma )</th>
<th>( \theta )</th>
<th>Plane</th>
<th>( \gamma_{\text{app}} )</th>
<th>( \gamma_{\text{comp}} )</th>
<th>( \gamma_{\text{dil}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>33a</td>
<td>20.05</td>
<td>(143)</td>
<td>1044</td>
<td>1028</td>
<td>1028</td>
</tr>
<tr>
<td>19</td>
<td>26.53</td>
<td>(133)</td>
<td>702</td>
<td>695</td>
<td>695</td>
</tr>
<tr>
<td>27</td>
<td>31.59</td>
<td>(255)</td>
<td>-</td>
<td>-</td>
<td>980</td>
</tr>
<tr>
<td>9</td>
<td>38.94</td>
<td>(122)</td>
<td>786</td>
<td>649</td>
<td>649</td>
</tr>
<tr>
<td>11</td>
<td>50.48</td>
<td>(233)</td>
<td>-</td>
<td>-</td>
<td>730</td>
</tr>
<tr>
<td>33b</td>
<td>58.99</td>
<td>(455)</td>
<td>-</td>
<td>-</td>
<td>660</td>
</tr>
<tr>
<td>3</td>
<td>70.53</td>
<td>(111)</td>
<td>30</td>
<td>1.06</td>
<td>30</td>
</tr>
<tr>
<td>17</td>
<td>86.63</td>
<td>(433)</td>
<td>853+654E_0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>17*</td>
<td>93.37</td>
<td>(322)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>109.47</td>
<td>(2T1)</td>
<td>933+327E_0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>33b*</td>
<td>121.47</td>
<td>(522)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>11</td>
<td>129.52</td>
<td>(3T1)</td>
<td>1092+654E_0</td>
<td>1015+327E_0</td>
<td>-</td>
</tr>
<tr>
<td>9</td>
<td>141.06</td>
<td>(4T1)</td>
<td>1077+654E_0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>27*</td>
<td>148.41</td>
<td>(511)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>19*</td>
<td>153.47</td>
<td>(611)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>33a*</td>
<td>159.95</td>
<td>(811)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

According to the arbitrariness of the origin of the coordinate system various CSL may be constructed with the same unit cell but different grain boundary structures and only an energy calculation can show which CSL (for a given rotation angle \( \theta \) ) yields the boundary with the lowest energy. The different CSL can be transformed into each other by a translation vector. So it is a special property of the [011] rotation that the same CSL can also be created by a rotation of \( \phi = 180 - \theta \) and a relative shift of the two lattices by \( \frac{a}{4} <111> \).
Grain boundary studies in cubic metals have shown that certain low energy atomic configurations ("structural units") which have been identified in low energy CSL boundaries are also found in arbitrary boundaries. Close to a coincidence orientation the CSL structure is maintained by the incorporation of appropriate dislocation networks, at larger deviations the structure is made up by a mixture of structural units of neighboring CSL boundaries (eventually plus some dislocations and/or steps). Experimental results in semiconductors point towards the same direction. Therefore it seems necessary to get an overview of the possible relative lattice translations (and Burgers vectors) that maintain a certain grain boundary structure. Bollmann has shown that for each O-lattice a DSC lattice may be constructed that meets this condition. For the [011] rotation under consideration here it can be described by a body centered orthorhombic unit cell with

$$d_1 = \frac{1}{2} [k_2 2k_1 0]_{\text{tet}}$$

$$d_2 = \frac{1}{2} [k_1 k_2 0]_{\text{tet}}$$

Dislocations in CSL boundaries whose Burgers vector $b$ is not from the corresponding DSC lattice destroy the structure and must be connected with a structural fault.
Geometrical models were constructed for the CSL orientations of table 1 [9]. For the following considerations two typical structures will be presented here, the structure of a \( \Sigma = 33 \) (Fig. 3) and of a \( \Sigma = 11 \) (Fig. 4) boundary.

![Diagram](image1)

**Fig. 3:** \([011]\) projection of the \((\Sigma = 33)\) symmetric tilt boundary, \( \theta = 20.05^\circ \).

![Diagram](image2)

**Fig. 4:** \([011]\) projection of the \((\Sigma = 11)\), symmetric tilt boundary, \( \theta = 129.52^\circ \).

The first boundary contains no dangling bonds and consists of an array of structural units - a seven and five membered ring of atoms - which has been identified as a Lomer dislocation with a Burgers vector \( b = \frac{\sqrt{3}}{2} [011] \) and a \((100)\) glide plane. Since all of the CSL boundaries in the range \( \theta < 70.53^\circ \) \((\Sigma = 3)\) with \( \Sigma = 1 + 2n^2 \) \((n = 2 - 4)\) contain the same type of defect at different spacings, it has been proposed [9] that even arbitrary boundaries in this misorientation range can be built from this edge dislocation, a point which will be investigated later.

The structures of the CSL boundaries with \( \theta > 70.53^\circ \) all contained broken bonds, however, a possible reconstruction of bonds along the
[011] axis has to be taken into account.

On the basis of some of the proposed models computer calculations of the grain boundary energy were carried out. Since it is a special property of the covalently bonded materials that the wave functions forming a bond are strongly localized computations demand that one has to determine in advance how the atoms are connected with each other. The procedure described next therefore does not alter the essential features of a structure unless one begins from a different model.

2. Calculation of grain boundary energies.

2.1 Boundaries with no broken bonds.- The method used for the energy calculation has been derived earlier [12] and applied successfully to the determination of the core structure of dislocations in germanium and silicon [4,5,13]. It uses a pair potential function which allows the computation of the interaction energy of an atom with its four neighbors in the deformed crystal. Keating has derived the following approximation [14].

\[ E_{\text{harm}} = \frac{3a}{16r_o^2} \sum_{i=1}^{4} (r_{i1} - r_{20}^2) + \frac{2a}{8r_o^2} \sum_{i,j=1}^{4} (r_{i1} + r_{j1} - \frac{1}{3}r_{20}^2)^2 \]

This expression takes into consideration small deviations of the equilibrium distance \( r_o \) of two atoms and distortions of the equilibrium bond angles (second term, \( r_i \) difference vector between the atom and its \( i \)-th neighbor). It contains two free parameters \( (\alpha, \beta) \) which have to be fitted to the elastic moduli of the material. Since large deformations of bond angles and distances are to be expected in the vicinity of the boundary plane anharmonic terms have to be added to improve the calculations. A modified form of Keating's anharmonic potential developed by Koizumi and Ninomiya has finally been used [15].

\[ E = E_{\text{harm}} + \frac{3a}{16r_o^2} \sum_{i=1}^{4} (r_{i1} - r_{20}^2) \exp \frac{4\sqrt{3}\gamma}{3a r_o} (r_{i1} - r_{20}^2) \]

\[ + \frac{3\beta}{8r_o^2} \sum_{i,j=1}^{4} (r_{i1} + r_{j1} - \frac{1}{3}r_{20}^2)^2 \exp \frac{2\sqrt{3}\epsilon}{3a r_o} (r_{i1} + r_{j1} - 2r_{20}^2) \]

\[ + \frac{\sqrt{3}\delta}{2r_o^3} \sum_{i,j=1}^{4} (r_{i1} + r_{j1} - \frac{1}{3}r_{20}^2)^3 \]

That introduces three more parameters \( (\gamma, \delta, \epsilon) \) which are determined from the elastic modulus of the third order. They are given in reference [14,15] for germanium and silicon.

The total energy of a given assembly of atoms is the sum of the interaction energies of all atoms. For the beginning atoms far away from the boundary plane were fixed whereas all other atoms were shifted in the direction of the largest energy gradient until the minimum configuration was reached. Usually it was sufficient to relax only a few atoms in the vicinity of the boundary. In a second step relative translations of the two crystal lattices perpendicular and parallel to the boundary plane were introduced. For the symmetric boundary structures (\( \Sigma = 33, 19, 3 \)) only translations perpendicular to the boundary plane were necessary to reach the equilibrium configuration whereas for the asymmetric structure of the \( \Sigma = 9 \) boundary [7,9] also
a small displacement of about 5% of the periodicity length parallel to the plane was needed. The computed relative energies (related to the area of the plane) \( \gamma_{\text{comp}} \) are given in table 1.

The calculations show that the relaxation of the atoms reduces the total energy by about 40%. Earlier Müller [9] has approximated the boundary energies by just taking into account the energy of the bonds which connect the crystals

\[
E_{\text{app}} = n E_0 + E_1 \sum \sin^2 \alpha_i
\]

where \( E_0 \) is the mean energy of a broken bond, \( n \) their number, \( \alpha_i \) the distortion angle of the \( i \)-th bond in the boundary plane. The second term of this equation is derived from the elastic shear energy per unit volume with \( E_1 = 7.2 \, \text{eV} \) for silicon, however, does not take into account atom relaxation. If one reduces \( E_1 \) by about 40% one yields surprisingly similar values to the computer calculated boundary energies (table 1). With this adjusted parameter \( E_1 \), the energies of some of the remaining grain boundaries were approximated.

2.2 Boundaries with broken bonds.- The geometric model of the \( \Sigma = 11 \) boundary (Fig. 4) shows a structure with two bonds per periodicity length. The dangling bonds point either up- or downwards. The energy calculation of structures with an isolated bond was performed in the following way. The single bond was saturated by an atom which was allowed to adjust so that the distortion energy of this bond could be kept as small as possible. The total energy is then the sum of the minimized boundary energy plus the energy of a dangling bond \( (= E_0/2) \).

Unfortunately there is still a great uncertainty as to the absolute value of \( E_0 \); Marklund [5] gives \( E_0 = 1 \, \text{eV} \), Jones [4] \( E_0 = 2 \, \text{eV} \) and Müller [9] \( E_0 = 1.8 \, \text{eV} \). Therefore in some cases it may be impossible to decide which reconstructed structure has to be favored.

For \( \Sigma = 11 \) two possibilities of reconstructing the dangling bonds were tested, a partial saturation of every second bond in the symmetry planes of the boundary along the [011] direction and an alternating arrangement of the remaining dangling bonds, and the total reconstruction of all bonds. Table 2 gives the results for silicon which show that in any case the partial reconstruction yields the lowest energy.

<table>
<thead>
<tr>
<th>Reconstruction</th>
<th>( \gamma_{\text{comp}} ) [erg/cm(^2)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>no reconstruction</td>
<td>1238 + 327 (2( E_0 ))</td>
</tr>
<tr>
<td>partial reconstruction</td>
<td>1015 + 327 (1( E_0 ))</td>
</tr>
<tr>
<td>total reconstruction</td>
<td>1837 + 0 ( E_0 )</td>
</tr>
</tbody>
</table>

3. Energy of periodic dislocation arrays.- It is tempting to treat all symmetric grain boundaries in the angular range \( 0 \leq 38.94^\circ (\Sigma = 9) \) as an array of Lomer edge dislocation as has been suggested earlier. That should be possible because the Burgers vector \( \mathbf{b} = \frac{2}{3}[011] \) is a crystal lattice vector and therefore belongs to the DSC lattices which can be constructed for each orientation angle \( 0 \).

Since the Read and Shockley equation [17] for the energy (per unit area) of a small angle boundary is an approximation for small angles \( (0 \lesssim 10^\circ) \) one first has to generalize the equation in order to compare with computer calculated CSL boundary energies.
Let us consider therefore the periodic array of edge dislocations of Fig. 5, which form a symmetric tilt boundary. For larger angles one cannot neglect anymore that both lattices are tilted away from the boundary plane by $\theta/2$ and accordingly the same is true for the dislocations and their Burgers vector. The different spacings $D_0$ and $2D$ are introduced here to account also for boundaries with not evenly spaced dislocation arrays (e.g. $\Sigma = 33$). The energy (per unit area) $\gamma_{\text{disl}}$ stored in such a dislocation array has been calculated following a procedure given in [18]. It yields

$$
\gamma_{\text{disl}} = \gamma_0 \sin \theta/2 \left\{ \cos^2 \frac{\theta}{2} \left[ \eta_o \coth \eta_o - \ln(2\sinh \eta_o) \right] + \sin^2 \frac{\theta}{2} \left[ \eta_o/\sinh \eta_o + \ln \tanh \eta_o/2 \right] \right\} + \gamma_c
$$

with $\gamma_0 = \mu b/2\pi(1-\nu)$, $\eta_o = (2\pi \sin \theta/2)/b$, $\nu$ Poisson's ratio and $r$ the core radius of the edge dislocation.

If the dislocations are not evenly spaced then $\gamma_c$ is not zero and becomes

$$
\gamma_c = \frac{1}{2} \gamma_0 \sin \theta/2 \left\{ \ln \frac{\cosh \eta_o + 1}{\cosh \eta_o - \cos \theta} + \eta_o \frac{(1+c)(\cos \theta \cosh \eta_o - \cos^2 \theta + 1)}{\sinh \eta_o (\cosh \eta_o - c)} \right\}
$$

where $c = \cos \pi D_0/D$.

Equations 7,8 contain two parameters $\gamma_0$ and $r$, if we consider $\gamma_0$ a free parameter for the beginning. Fitting this equation to the computer calculated grain boundary energies of $\Sigma = 33, 19$ and $9$ we obtain the following values (table 3).

Table 3.- Comparison of computer calculated grain boundary energies and energies of periodic dislocation arrays. All energies in [erg/cm²].

<table>
<thead>
<tr>
<th>$\Sigma$</th>
<th>$\gamma_{\text{comp}}$</th>
<th>$\gamma_0$</th>
<th>$r/b$</th>
<th>$\mu b/2\pi(1-\nu)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>33</td>
<td>1028</td>
<td>4920</td>
<td>0.51</td>
<td>4920</td>
</tr>
<tr>
<td>19</td>
<td>695</td>
<td>4920</td>
<td>0.51</td>
<td>4920</td>
</tr>
<tr>
<td>9</td>
<td>649</td>
<td>4920</td>
<td>0.51</td>
<td>4920</td>
</tr>
<tr>
<td></td>
<td>4820</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The comparison shows an excellent agreement between the fitted parameter $\gamma_0$ and the value of $\mu b/2\pi(1-\nu)$ if one uses the Burgers vector of the dislocation $b=a/2[011]$. The value $r=0.5b$ for the cut-off radius is reasonable. Although the dislocation cores begin to overlap for $\theta \geq 26.53$ ($\Sigma = 19$) the equation (7) still seems to be valid for larger angles, however, a slightly reduced core radius results in the case of the $\Sigma = 9$ boundary.

Fig. 5
With the help of equation 7 and the values for $\gamma_0$ and $r/b$ one is able now to calculate energies of more periodic dislocation grain boundaries. Two types of spacings have been considered ($n \geq 3$)

(a) with $D_0/D = n/n+1$ if $n$ is odd,
(b) and $D_0/D = 1$ if $n$ is even.

In both cases we have a CSL boundary with $\Sigma = 1+2n^2$ and $\theta = 2 \arctan 1/n/\sqrt{2}$. The calculated energies are given in Fig. 6.

The energies calculated here are valid for temperatures $T = 0$. In order to compare with experimentally determined values one has to take into account, that the entropy of the boundary is likely to reduce the energy of an arbitrary boundary more than that of a more perfect CSL boundary. Therefore free energy curves versus misorientation $\theta$ are smoothed out and only deep cusps in the $\gamma(\theta)$ curve are expected to remain, in our case probably the cusps at $\theta(\Sigma = 19,9$ and 3).

We may also consider the structure of the grain boundaries treated so far as a mixture of structural units of the adjacent CSL boundaries, in our case the perfect lattice structure and the $\Sigma = 19$ structure (Lomer dislocation). The question arises whether it may also be possible to construct boundary structures in the angular range $38.94 < \theta < 70.53$ in the same manner.

An arbitrary angle of $\theta = 50^\circ$ has been chosen and it can actually been shown (Fig. 7) that the structure is a mixture of the Lomer dislocation structure with the stacking fault structure of the twin boundary. From equation 7 it is again possible to calculate the energy of the periodic dislocation array. The result is given in Fig. 6 for ($n \geq 0$)

(a) $D_0/D = (3+n)/(4+n)$ if $n$ is even
(b) $D_0/D = 1$ if $n$ is odd,
and $\theta = 2 \arctan ((2+n)/(4+n)\sqrt{2})$.

We have demonstrated that at least for the [011] tilt boundary with $\theta \leq 70.53$ the boundary structures can either be treated as a dislocation array or as a mixture of structural units of neighboring CS lattices. The latter view seems more appropriate if one takes into account results gained from the study of grain boundaries in cubic metals.
References


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[16] READ W.T., SHOCKLEY W., Phys. Rev. 78 (1950) 275


DISCUSSION

M. HEGGIE.- The Keating potential cannot be fitted to phonon dispersion curves throughout the Brillouin zone. The values of the Keating parameters vary by up to a factor 3 between different authors. How can you place confidence in your calculations?

H.J. MÖLLER.- The set of parameters used was the one which is most appropriate for these kind of calculations. Unpublished results by H. Veth on the core structure of dislocations in germanium and silicon showed quite good agreement with experiments.

R.C. POND.- Have you considered the possibility of removing individual atoms from grain boundary structures in order to reduce their energy. In materials with a double atom basis this type of relaxation leads to structures which cannot be obtained alternatively by relative displacement.

H.J. MÖLLER.- Yes, this has been considered in general. However, no comparative calculations for a specific structure have been carried out yet.
H.F. MATARÉ.- Which portion of the energy is more important within your calculation of the cusps: lattice reconstruction (no dangling bonds) or lowered strain energy? In the Read-Shockley energy envelope, we generally interpreted cusps as due to twin relations or mainly to elimination of dangling bonds.

H.J. MÖLLER.- The calculation of Σ11 grain boundary energy shows that a bond reconstruction can raise the strain energy considerably and therefore may be unfavorable. In general both portions of the energy are equally important and only the detailed calculation can show what structure occurs.