



HAL
open science

ELASTIC ENERGY OF FACETED LOW ANGLE TILT BOUNDARIES

D. Divincenzo

► **To cite this version:**

D. Divincenzo. ELASTIC ENERGY OF FACETED LOW ANGLE TILT BOUNDARIES. Journal de Physique Colloques, 1985, 46 (C4), pp.C4-243-C4-248. 10.1051/jphyscol:1985427 . jpa-00224677

HAL Id: jpa-00224677

<https://hal.science/jpa-00224677v1>

Submitted on 4 Feb 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

ELASTIC ENERGY OF FACETED LOW ANGLE TILT BOUNDARIES

D.P. DiVincenzo

*Laboratory of Atomic and Solid State Physics, and Materials Science Center,
Cornell University, Ithaca, NY 14853, U.S.A.*

Abstract. A closed form expression for the elastic energy of an arbitrary small angle tilt boundary is derived and used to study grain boundary faceting in NiO. Results are in good agreement with experiment. It is found that the rules of the O-lattice model, which is also successful in explaining the boundary structure in NiO, may be justified by and derived from the present elastic energy formalism.

I. INTRODUCTION

It was shown many years ago that a small angle grain boundary may be modeled in a geometrically and physically sensible way by an array of dislocation lines[1]. Historically, this description was first used for the simplest possible boundaries; for example, the symmetrical small angle tilt boundary was shown[1] to consist of a set of identical, coplanar, parallel edge dislocations. The situation is not quite as simple in the case of lower-symmetry tilt boundaries where the interface lies along a high Miller index plane, which have recently been studied by electron microscopy[2]. For these boundaries Frank's formula[3] requires that more than one type of dislocation be present in the boundary, and there is no symmetry condition requiring the dislocation array to be planar; indeed, the dislocations in these boundaries are observed to assume a faceted structure[2].

An explanation for this faceting geometry has been constructed using the O-lattice model[4]. This model finds the points of "best match" between the two crystals (the O-points, or O-lines) by a geometrical construction, then postulates that the boundary dislocations will occur midway between the O-points. This model has successfully obtained the faceting structures as seen in experiment[2]. The O-lattice model is incomplete, however, in that it does not address the question which arises naturally within linear elasticity theory: are the grain boundary dislocations in elastic equilibrium? In other words, are the dislocations in positions which minimize the elastic energy of the boundary?

In this paper I will answer these questions by an exact evaluation of the energy of an arbitrary small angle tilt boundary within linear elasticity theory. This calculation goes beyond the O-lattice theory by providing a genuine prediction of grain boundary structure, not just a geometrically-inspired guess. In the cases considered below, it is found that the O-lattice model predicts dislocation positions which are very nearly (although not precisely) in elastic equilibrium. As will be discussed below, the O-lattice model obeys some simple rules that are derivable from linear elasticity theory, which allow it to give sensible predictions for most cases.

In the remainder of the paper I will examine in detail two faceted tilt boundaries which have been studied in NiO: one with a tilt axis in the [001] direction, the other in the [209] direction. NiO is an fcc ceramic; however, the theory to presented is quite general and applies to any isotropic solid.

II. FORMALISM

Dislocations are well-defined topological entities in linear elasticity theory, singularities which arise from the multi-valuedness of the lattice displacement field. They produce certain

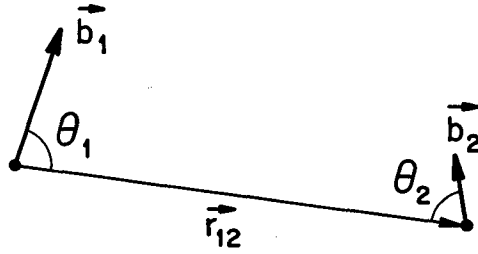


Fig.1. Two parallel dislocations with Burgers vectors \vec{b}_1 and \vec{b}_2 separated by \vec{r}_{ij} . The two dislocations have the lowest interaction energy when $\theta_1 = \theta_2$.

unique stress and strain fields in the elastic medium. Since stress times strain is energy, their presence changes the energy density of the medium in an exactly calculable way. If the medium contains two dislocations i and j, the resulting stress and strain fields in the medium are, in the linear approximation (which is correct so long as the dislocation cores do not overlap), simply given by the superposition of the fields emanating from the two dislocations. From this the energy density and the resulting energy of interaction V_{ij} may be computed. Consider two straight parallel dislocations (Fig. 1) running along direction $\hat{\xi}$, (i.e., out of the paper), one with Burgers vector \vec{b}_1 at position \vec{r}_1 , the other with Burgers vector \vec{b}_2 at position \vec{r}_2 . The \vec{b} 's must be lattice vectors of the crystal, but they may have a component pointing into (or out of) the plane of Fig. 1. It is assumed here that $\hat{\xi} \cdot \vec{r}_{12} = 0$. The resulting interaction energy is [5,6]:

$$V_{12} = -K \vec{B}_1 \cdot \vec{B}_2 \ln |\vec{r}_1 - \vec{r}_2| + K \frac{\vec{B}_1 \cdot \vec{r}_{12} \vec{B}_2 \cdot \vec{r}_{12}}{|\vec{r}_{12}|^2} \tag{1}$$

\vec{B} is related to \vec{b} by $\vec{B} \equiv \sqrt{1-\nu} \hat{\xi} (\vec{b} \cdot \hat{\xi}) + \hat{\xi} \times (\vec{b} \times \hat{\xi})$ (amounting to a compression of the coordinate system along the dislocation axis $\hat{\xi}$), and $K \equiv \mu / 2\pi(1-\nu)$. Here μ is the shear modulus and ν is the Poisson ratio.

I have used the isotropic approximation, in which the elastic constants of the solid are assumed to be related by $2c_{44} = c_{11} - c_{12}$; this condition is reasonably well satisfied in NiO, for which [7] $\mu = 0.97 \times 10^{12}$ dyn/cm² and $\nu = 0.27$. The results below are rather insensitive to the actual values of these elastic constants, and so it seems likely that the isotropic approximation itself is not very crucial. Note that Eq. (1) is only determined to within an additive constant, which is usually absorbed within an (unknown) core radius and core energy. The expression given above actually differs from that given on p.117 of [5] by an additive constant $K(\hat{\xi} \times (\vec{b}_i \times \hat{\xi})) \cdot (\hat{\xi} \times (\vec{b}_j \times \hat{\xi}))$. This will not affect the analysis below, where I will only be concerned with the relative energy of two different configurations.

In a pure tilt boundary (in which the direction of the rotation axis $\hat{\theta}$ lies in the boundary plane) all dislocation lines are parallel to the $\hat{\theta}$ axis. A general small angle tilt boundary is illus-

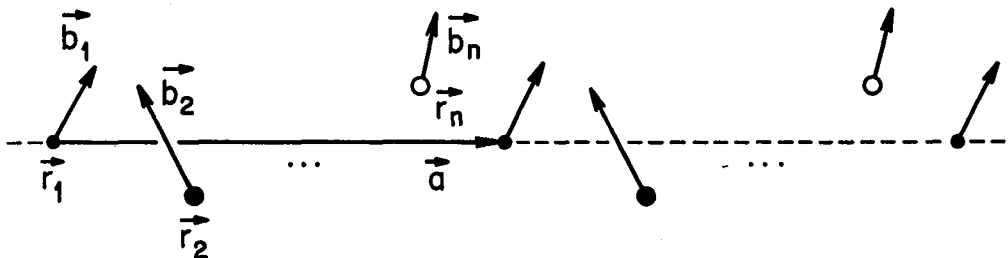


Fig.2. A general small angle tilt boundary. The different symbols represent dislocations with Burgers vectors $\vec{b}_1, \vec{b}_2, \dots$ at positions $\vec{r}_1, \vec{r}_2, \dots$. The structure of the boundary is assumed to be periodic with period vector \vec{a} with n dislocations per period.

trated in Fig. 2, with dislocations at positions $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n$ with Burgers vectors $\vec{b}_1, \vec{b}_2, \dots, \vec{b}_n$. The dislocation structure of the boundary is assumed to be periodic with period \vec{a} . Note that the dislocations need not lie in the same plane as \vec{a} . The dislocation content of the boundary is not entirely arbitrary, however; it must satisfy a geometrical constraint, Frank's formula[3,5]: $\sum_{i=1}^n \vec{b}_i = \vec{a} \times \vec{\theta}$. Within this constraint, however, a wide variety of dislocation configurations are possible. To decide among them, I will minimize the energy of the array of dislocations as a function of their positions $\{\vec{r}_i\}$ using the formula above. One might think of writing the energy per unit area of the boundary as $E = 1/a \sum_i E_i^{core} + 1/2a \sum_{ij} V_{ij}$, where E^{core} is the core energy of the dislocation. Unfortunately, this expression as written is divergent because of the arbitrary (and unknown) constant in V_{ij} mentioned above. This problem is solved by *defining* a particular reference boundary to have zero energy, say the one for which the dislocation positions are \vec{r}_i^0 .

The energy *difference* between the reference boundary and the boundary of interest,

$$E = \frac{K}{2a} \sum'_{i,j=1}^n \sum_{k=-\infty}^{\infty} \left[-\vec{B}_i \cdot \vec{B}_j \ln |\vec{r}_i - \vec{r}_j - k\vec{a}| + \frac{\vec{B}_i \cdot (\vec{r}_i - \vec{r}_j - k\vec{a}) \vec{B}_j \cdot (\vec{r}_i - \vec{r}_j - k\vec{a})}{(\vec{r}_i - \vec{r}_j - k\vec{a})^2} + \right. \\ \left. \vec{B}_i \cdot \vec{B}_j \ln |\vec{r}_i^0 - \vec{r}_j^0 - k\vec{a}| - \frac{\vec{B}_i \cdot (\vec{r}_i^0 - \vec{r}_j^0 - k\vec{a}) \vec{B}_j \cdot (\vec{r}_i^0 - \vec{r}_j^0 - k\vec{a})}{(\vec{r}_i^0 - \vec{r}_j^0 - k\vec{a})^2} \right] \quad (2)$$

is a well converged quantity, and can be used to look for equilibrium geometries of boundary structures by minimizing E. The infinite sum over unit cells k in Eq. (2) can actually be evaluated in closed form; the result, after some tedious algebra, is

$$E = -\frac{1}{4} \frac{K}{a} \sum'_{ij} \vec{B}_i \cdot \vec{B}_j \ln \left[\frac{\cosh(2\pi\epsilon_{ij} \sin\theta_{ij}) - \cos(2\pi\epsilon_{ij} \cos\theta_{ij})}{\cosh(2\pi\epsilon_{ij}^0 \sin\theta_{ij}^0) - \cos(2\pi\epsilon_{ij}^0 \cos\theta_{ij}^0)} \right] + E_2 - E_2^0 \quad (3)$$

$$E_2 \equiv \frac{1}{2} \frac{K}{a} \sum'_{ij} \left\{ \frac{\pi}{\epsilon_{ij} \cos\theta_{ij} \sin\theta_{ij} [\tan^2(\pi\epsilon_{ij} \cos\theta_{ij}) + \tanh^2(\pi\epsilon_{ij} \sin\theta_{ij})]} \times \right. \\ \left[\cos\theta_{ij} \tanh(\pi\epsilon_{ij} \sin\theta_{ij}) \sec^2(\pi\epsilon_{ij} \cos\theta_{ij}) (D_i D_j - A_i A_j \epsilon_{ij}^2 + 2A_i D_j \epsilon_{ij} \cos\theta_{ij} + 2A_i A_j \epsilon_{ij}^2 \cos^2\theta_{ij}) - \right. \\ \left. \left. 2\sin\theta_{ij} \tan(\pi\epsilon_{ij} \cos\theta_{ij}) \operatorname{sech}^2(\pi\epsilon_{ij} \sin\theta_{ij}) (A_i D_j \epsilon_{ij} \cos\theta_{ij} + A_i A_j \epsilon_{ij}^2 \cos^2\theta_{ij}) \right] \right\} \quad (4)$$

Here $\vec{r}_{ij} \equiv \vec{r}_{ij}/a$, $\vec{r}_i \equiv \vec{r}_i - \vec{r}_j$, $D_i \equiv \vec{B}_i \cdot \vec{r}_{ij}$, $A_i \equiv \vec{B}_i \cdot \vec{a}/a$, and $\cos\theta_{ij} \equiv -\vec{a} \cdot \vec{r}_{ij}/a r_{ij}$. Also, E_2^0 is the same as E_2 with \vec{r}_i replaced by \vec{r}_i^0 , θ_{ij} replaced by θ_{ij}^0 , etc. Despite the complexity of this formula, its evaluation on a computer is quite straightforward. Thus, the strategy for any particular boundary of interest is simply to find the positions $\{\vec{r}_i\}$ which minimize the boundary energy E in Eq. (3) for a particular set of dislocations $\{\vec{b}_i\}$.

III. [001] BOUNDARY

Figure 3 shows the dislocation structure as observed by electron microscopy[2] in a $\theta \approx 1^\circ$ tilt boundary in NiO. The tilt axis is along the low-index direction [001], but the boundary plane itself is not a low Miller index plane, and the boundary period vector \vec{a} (dashed line in Fig. 2) points away from the [110] direction by $\sim 3.6^\circ$. Thus it is not possible to satisfy Frank's formula with only one type of fcc Burgers vector; it can be satisfied, however, if the boundary period contains eight $1/2[110]$ dislocations for every one $1/2[110]$ dislocations. Since the boundary period is observed to contain nine dislocations, this would seem a reasonable hypothesis. A boundary structure which is consistent with the O-lattice model[2] would place the eight $1/2[110]$ in a single facet lying precisely along the [110] (median) direction, with the $1/2[110]$ dislocation lying in a step, with $\phi = 45^\circ$. The points in Fig. 4 show this O-lattice prediction for one period of the boundary in Fig. 3.

This structure is in reasonable agreement with experiment, so I have taken the O-lattice structure to be the reference configuration (see Eq. (2) above) in a dislocation energy calculation.

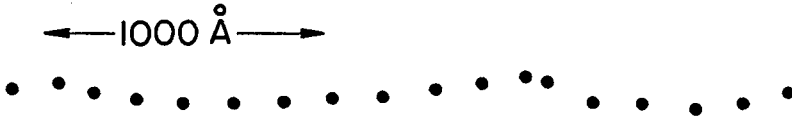


Fig.3. The dislocation structure as seen in electron microscopy[2,8] of a $\theta=[001]$ tilt boundary in NiO. Note the faceted arrangement of the dislocations.

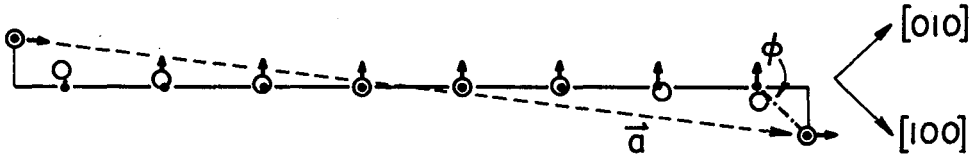


Fig.4. One period of the boundary in Fig. 3. \vec{a} is shown as a dashed line, and the arrows show the Burgers vectors of the dislocations. In the O-lattice model (solid points) the dislocations lie exactly on the solid lines and $\phi=45^\circ$. In the fully relaxed configuration of the present calculation (open circles) the facet is significantly rounded.



Fig.5. The dislocation structure as seen in electron microscopy[2,8] of a $\theta=[\bar{2}09]$ tilt boundary in NiO. Note the two different spot sizes, which is indicative of Burgers vectors of two different lengths. The dashed line encloses a defect in the faceting structure of the boundary.

When I permit these dislocations to relax to their minimum energy state, they assume the configuration shown as the open circles in Fig. 4. The deviation from the O-lattice configuration is fairly small. The qualitative features of the faceting is preserved, and the energy gained by relaxation from the O-lattice positions, ~ 1.0 erg/cm², is on the order of a percent of the estimated value of the total interfacial energy[5], 300erg/cm². Rather than perfectly straight as in the O-lattice model, the ends of the facet are predicted to be significantly rounded, with dislocation positions being as much as 10Å from the facet line; however, disorder in the experimentally observed structure (Fig. 3) causes both the O-lattice result and the dislocation energy result to be equally plausible. Different sample preparation (e.g., longer anneal times) may permit an observation of this rounding, which would be an important confirmation of the grain boundary dislocation model.

IV. $[\bar{2}09]$ BOUNDARY

Figure 5 shows the dislocation structure, as observed in electron microscopy, of another tilt boundary in NiO[2]. Here the tilt angle $\theta \approx 12.25^\circ$, the tilt axis $\theta=[\bar{2}09]$, and the boundary period vector \vec{a} lies about 6° from the $[010]$ direction. This boundary is more complicated than the one above; for this geometry *three* different types of Burgers vectors are required to satisfy Frank's formula. Also, the variation in the observed contrast of the dislocations in Fig. 5 suggests that dislocations with Burgers vectors of at least two different lengths occur. A set of dislocations consisting of three $[100]$ dislocations (A), two $1/2[101]$ dislocations (B), and one $1/2[110]$ dislocation (C), will satisfy Frank's formula in this case. Since the observed boundary period actually contains six dislocations, three with heavy contrast, this dislocation set seems to

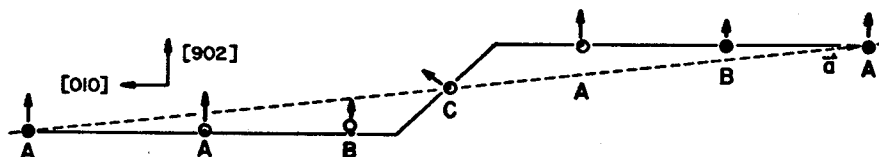


Fig. 6. Theoretical analysis of the circled region of Fig. 5. The boundary contains dislocations with three different Burgers vectors (arrows): A ($[100]$), B ($1/2[101]$), and C ($1/2[110]$). The fully relaxed positions (open circles) are very close to the O-lattice positions (points).

be a plausible hypothesis. The O-lattice model[2] provides a possible dislocation structure which agrees closely with experiment, in which five of the dislocations lie in a straight facet along the $[010]$ direction, with the lone $1/2[110]$ lying in a step; this configuration is shown as the points in Fig. 6, which represents the circled region of the boundary in Fig. 5.

Again I have used the O-configuration as the reference structure in the energy calculation of Eq. (3) and determined the equilibrium configuration of the dislocations in the boundary. The resulting structure, shown as the open circles in Fig. 6, is very close to O-lattice model (the difference is probably less than the available experimental resolution), and the gain in boundary energy from the O-lattice to the fully relaxed geometry is only 2.2erg/cm^2 , just a fraction of a percent of the estimated interfacial energy[5] of 2000erg/cm^2 . A wide variety of other possible reconstruction geometries have been studied, and although other metastable states occur, the structure shown in Fig. 6 has the lowest energy. Thus in this case the O-lattice model is successful in predicting the equilibrium structure of the boundary.

However, the present energy calculation is capable of giving more complete information about the actual structure of the grain boundary. For example, in the real boundary (Fig. 5) a defect occurs (dashed circle) in which the facet length changes from 5 to 8. Using a total energy calculation I have been able to confirm that this faceting fault is indeed a metastable configuration of the boundary, i.e., there is an energy barrier for it to annihilate with a length 2 facet and return to the ground state. Furthermore, the excess line energy of this defect can be computed and is found to be $\sim 8\text{meV/\AA}$, which is quite small on the scale of line energies of free dislocations in solids[5].

In addition to this, the dislocation energy calculation can provide information about the tendency of long Burgers vector dislocations (e.g., dislocation A in Fig. 6) to dissociate in the elastic energy calculation into two primitive dislocations. According to the "b-squared" criterion[8] (which should really be the "B-squared" criterion, with B defined below Eq. (1)), for small enough tilt angle the $[100]$ dislocations in this boundary *must* dissociate into $1/2[101]$ and $1/2[10\bar{1}]$ dislocations. However, this is only required to occur in the limit of vanishingly small tilt angle, and in other materials it has been shown[8] that the b-squared criterion need not be satisfied in the range of θ 's of practical interest ($\theta > 1^\circ$). In the present calculation, when a $[100]$ dislocation is permitted to dissociate in the $[209]$ boundary, the resulting dislocations equilibrate at a distance which is on the order of the core radius ($\sim 5\text{\AA}$); therefore, for all practical purposes the energy calculation predicts that the $[100]$ dislocations do not dissociate in this boundary.

V. DISCUSSION

An important question which the present energy calculations can answer is: why does the O-lattice model work so well for the cases considered? It should be understood that the O-model cannot give a unique prediction for boundary structure; it can only give a list of reasonable candidates, which can only be decided between by experiments or by energy calculations. For example, the O-lattice model can never determine the tilt angle at which the b-squared criterion will begin to be violated as in the $[209]$ boundary above. However, the O-lattice candidates which are shown in this paper for the observed $[100]$ and $[209]$ boundaries are very close to the true elastic equilibrium geometries, despite the fact the usual justification for the O-lattice predictions in terms of "best match" regions makes no reference to dislocation energetics.

The reason that the O-lattice works is that it unintentionally incorporates some of the simplest rules of interdislocation forces. It is a consequence of the energy expression Eq. (1) that the equilibrium orientation for a single pair of dislocations (see Fig. 1) for a fixed $|\vec{r}_{ij}|$ is achieved when $\theta_1 = \theta_2$. As Figs. 4 and 6 illustrate, the O-lattice rules conspire to satisfy this criterion. Another simple rule which comes out of the energy expressions is that screw components on neighboring dislocations should be of opposite sign as often as possible; this is embodied in the O-lattice rules for constructing the "stepped b-net" [2]. Still, this does not really explain why the O-prediction is as good as it is for the [209] boundary; from the point of view of the present calculation, this must be viewed as simply an accident.

In summary, I have obtained tractable, closed form energy expressions for the elastic energy of a general small angle tilt boundary in isotropic solids. This formalism has been applied to two faceted boundaries in NiO. The boundary geometries are accurately predicted by the theory; the facet structure is a simple consequence of the different Burgers vector dislocations which must occur in the boundary. The O-lattice model has also been successfully applied to these boundaries; the present work sheds some light on why the O-model actually works. However, the present energy calculations go beyond the O-lattice analysis by predicting the presence of metastable defects and ruling out dislocation dissociation in the [209] boundary.

I thank Dr. M. D. Vaudin and Profs. S. L. Sass, J. W. Wilkins, and N. W. Ashcroft for helpful discussions. This work is supported by the National Science Foundation through the Materials Science Center at Cornell University.

References.

1. See, e.g., W. T. Read, Jr., *Dislocations in Crystals* (McGraw-Hill, New York) 1953.
2. J. Eastman, F. Schmückle, M. D. Vaudin, and S. L. Sass, *Advan. Ceram.*, to be published; M. D. Vaudin, M. Rühle, and S. L. Sass, *Acta Metall.* **31** (1983) 1109.
3. F. C. Frank, in *Symposium on the Plastic Deformation of Crystalline Solids* (Carnegie Institute of Technology, Pittsburgh) 1950, p. 150.
4. W. Bollmann, *Crystal Defects and Crystalline Interfaces* (Springer Verlag, New York) 1970.
5. J. P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York) 1982.
6. F. R. N. Nabarro, *Theory of Dislocations* (Clarendon, New York) 1967.
7. N. Uchida and S. Saito, *J. Acoust. Soc. Am.* **51** (1972) 1602; P. de V. du Plessis, S. J. van Tonder, and L. Alberts, *J. Phys. C* **4** (1971) 1983.
8. A. H. King and D. A. Smith, *Acta Crystallogr. A* **36** (1980) 335; A. P. Sutton and V. Vitek, *Phil. Trans. Roy. Soc. Lond. A* **309** (1983) 1.