

AN EMPIRICAL MODEL OF GRAIN BOUNDARY ENERGY AND ITS APPLICATION TO GRAIN BOUNDARY WETTING

Wynblatt P. *, AND Takashima M.**

*Dept. of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh PA 15206, USA.

**Technical Research Labs, Kawasaki Steel Corporation, Kurashiki, 712-8511 Japan.

ABSTRACT

We present an analytical model of the dependence of grain boundary (GB) energy in terms of the 5 macroscopic degrees of freedom (DoF's) of GB character. The model is empirical in the sense that trends in GB properties have been constrained to follow the results of previous GB computer simulations. It is used in this paper to interpret the experimental wetting behavior of 975 GB's by liquid Cu in an Fe-30 wt% Mn-10 wt% Cu alloy, the character of which was determined by orientation imaging microscopy, in conjunction with serial sectioning. It is shown that the model correctly predicts the wetting behavior for over 80% of the GB's studied.

1. INTRODUCTION

With the advent of automated orientation imaging microscopy (OIM), it has become possible to determine various physical properties of sets of a thousand or more grain boundaries (GB's) as a function of the five macroscopic degrees of freedom (DoF's) of GB character [1,2]. In the near future, this experimental approach will make it possible to investigate sets which number in the tens of thousands of GB's. These developments far outstrip the modeling capabilities of GB properties by the very successful computer simulation approach which has evolved over the past several years [3-6].

The purpose of this paper is to present an empirical analytical model of GB energy over the five macroscopic DoF's of GB structure, and to apply it to the interpretation of recent experimental results on GB wetting [7-9]. The model is based on a nearest neighbor (NN) bond framework originally developed for describing the energy of surfaces of orientation (hkl), and is therefore not expected to produce results that are as realistic as those of computer simulations performed in conjunction with many-body interatomic potentials. Nevertheless, because of its analytical form, it provides an approach which can be applied much more readily to the interpretation of vast sets of GB data.

2. EXPERIMENTAL CHARACTERIZATION OF GB WETTING

We have recently determined the wetting behavior of 975 GB's in an Fe-30wt%Mn-10 wt%Cu alloy, as a function of the five macroscopic DoF's. The material was equilibrated at 1120°C, where it consists of about 5% of a Cu-rich liquid phase coexisting with an fcc Fe-rich solid solution, and quenched. The orientations of grains in micrographs such as Fig. 1 were obtained from electron backscattering patterns in an orientation imaging microscope and the GB inclinations were determined by serial sectioning. Each GB was categorized as being either wet, dry or mixed (i.e. partly wet and partly dry). For the present purposes, the mixed GB's were ignored. For reasons that will become clear below, we have chosen to describe the five macroscopic DoF's by the crystallographic orientations, $(hkl)_1$ and $(hkl)_2$, of the two surfaces terminating the grains on either side of the GB, and a twist angle, ϕ , of the terminating planes with respect to their normal [10]. Because of experimental uncertainties in the (hkl)

* Corresponding author. Paul Wynblatt, Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh PA 15213, USA. Fax: +1-412-268-7596, e-mail: pw01+@andrew.cmu.edu

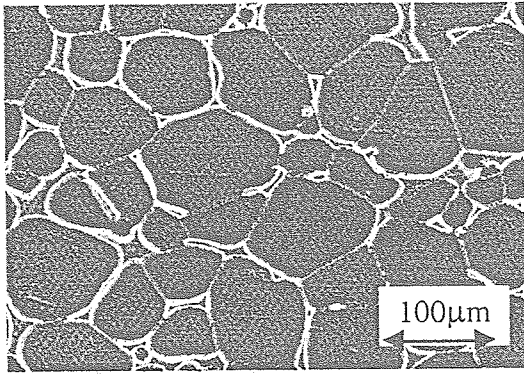


Figure 1. Example of SEM micrograph of Fe-Mn-Cu alloy used for characterizing wetting of GB's

values of both planes delimiting the GB's as well as the twist angle, the stereographic triangle has been subdivided into 10 segments, around the poles shown in Fig. 2. Details of the experimental procedures and of the methods used to calculate the five DoF's have been described previously [9], and will not be repeated here.

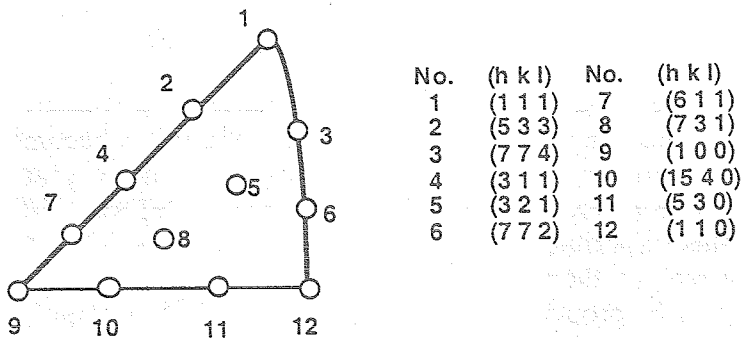


Figure 2. Stereographic triangle showing the 12 orientations which represent the poles of the bounding surfaces of the GB's studied.

3. BACKGROUND FOR MODEL OF GB ENERGY

3.1 Computer Simulations of Grain Boundaries

The proposed model is empirical in the sense that it attempts to reproduce some general trends in GB behavior which have been demonstrated by computer simulations. In particular, we will make use of the results reported by Wolf in a series of articles [11-13]. In these papers, the five macroscopic DoF's have also been described by the crystallographic orientations of the two surfaces delimiting the GB, and a twist angle.

We reproduce in Fig. 3 certain results obtained by computer simulation [13] which are used as the basis of the present model. Figure 3a shows a typical example of GB energy as a function of twist angle. Note that for a given pair of terminating planes, the GB energy remains essentially constant over a plateau which extends over most of the range of twist angle. It does, however, display cusps at the two ends of the twist angle range, which represent asymmetric tilt grain boundaries. Occasionally (though not shown in Fig. 3a) shallow cusps are also found at specific twist angles within the plateau range which correspond to special boundaries. Figure 3b shows that the plateau GB energy obtained from simulations depends approximately linearly on GB free-volume, and that this linear trend passes close to the origin. Figure. 3c illustrates the result that the mean GB energy from the plateau region of Fig. 3a varies approximately linearly with the mean surface energy of the two terminating planes (defined as $\bar{\gamma}_s = (\gamma_{s(hkl)_1} + \gamma_{s(hkl)_2})/2$), and that it intercepts the average surface energy axis at a finite value. Thus, while the simulations indicate that the grain boundary energy is approximately proportional to the free-volume of the boundary, it is *not* proportional to the mean energies of the surfaces which adjoin the boundary.

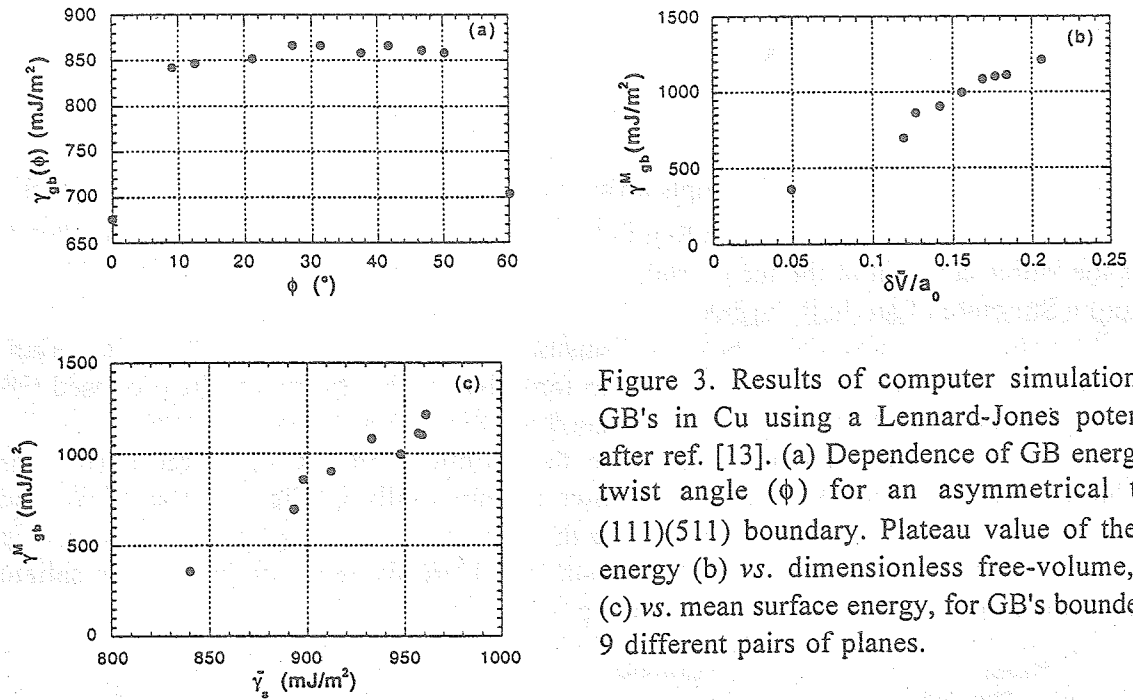


Figure 3. Results of computer simulations of GB's in Cu using a Lennard-Jones potential, after ref. [13]. (a) Dependence of GB energy on twist angle (ϕ) for an asymmetrical twist (111)(511) boundary. Plateau value of the GB energy (b) vs. dimensionless free-volume, and (c) vs. mean surface energy, for GB's bounded by 9 different pairs of planes.

3.2 Nearest Neighbor Bond Model of Surface Energy

We adopt the method of Lee and Aaronson [14] for calculating the energy of an fcc surface terminated by a plane of orientation (hkl). This approach uses the nearest neighbor bond model, and possesses features which are convenient for the present purposes.

For a surface of orientation (hkl) in an fcc crystal, it is convenient to choose a set of Miller indices that have been reduced to lowest possible integers, and for which $h \geq k \geq l$, such that all orientations fall within a stereographic triangle with corners at (100), (110) and (111). In such an (hkl) surface, atoms in the first J planes adjacent to the surface lack the full bulk coordination of $z=12$. Let the layers lacking neighbors be identified by an index i which ranges from 1 to J, where $i=1$ denotes the first surface layer, as shown schematically on the left hand side of Fig. 4. It is also necessary to define a second index, j, which counts planes from any plane i, as illustrated in the right hand side of Fig. 4. J is defined by:

$$J = \frac{1}{2}(h+k), \text{ for } h,k,l, \text{ all odd; and } J = (h+k), \text{ for } h,k,l, \text{ mixed.} \quad (1)$$

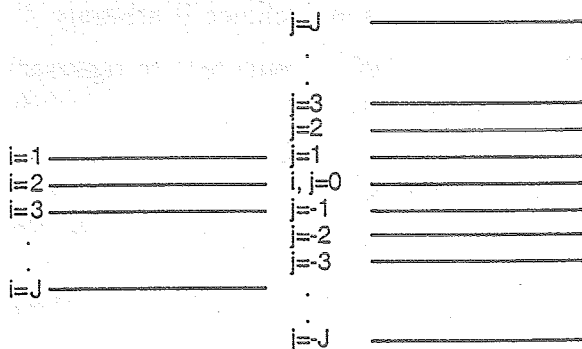


Figure 4. Schematic illustrating the definition of the indices i and j, for the case $i=2$.

In order to evaluate the surface energy, it is necessary to count the number of broken (missing) NN bonds of an atom in all planes $i = 1, 2, \dots, J$. This yields the result:

$$\gamma_{s(hkl)} = \frac{\alpha \epsilon}{a^2} \frac{1}{\sqrt{h^2+k^2+l^2}} \sum_{i=1}^J \sum_{j=i}^J z_j \quad (2)$$

where α is a geometric factor which adopts a value of 2 for hkl all odd and of 1 for mixed hkl , z_j is the number of broken bonds of an atom in the j th layer, ϵ is the energy of a broken bond, and a is the lattice constant of the fcc crystal.

3.3 Atomic Structure of an (hkl) Surface

The simulations described above demonstrate that GB free-volume is an important factor in the GB energy (see Fig. 3b). In order to formulate such a factor for the proposed GB model, we appeal to another description of free surfaces, due to Van Hove and Somorjai [15].

It has often proved useful to describe the atomic structure of a free surface as consisting of terraces, steps and kinks, as shown schematically in Fig. 5a. Van Hove and Somorjai have developed a method to determine the numbers of atoms present in terrace, step and kink sites, respectively, for any fcc (hkl) surface. Here we describe briefly the salient features of their approach, prior to its use in the present GB energy framework.

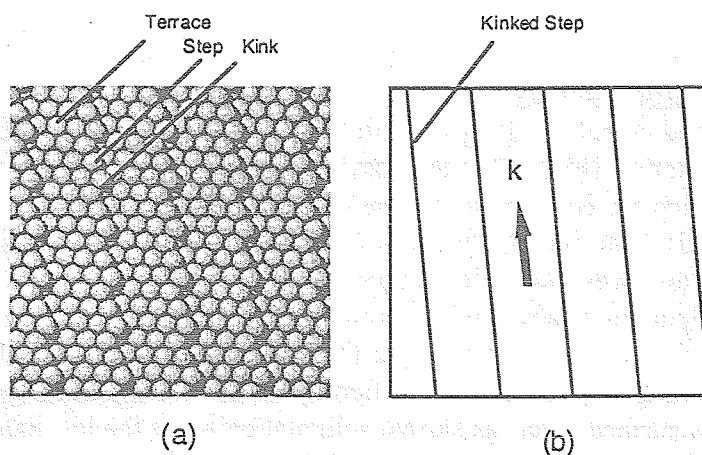


Figure 5. (a) Schematic of the structure of an fcc $(7\ 5\ 4)$ surface, showing terraces, steps and kinks, [downloaded from web site:

<http://www.aue.auc.dk/~stoltze>, with permission of Prof. Per Stolze]. (b) schematic showing the mean direction of kinked steps on the surface.

As in the Lee and Aaronson model [14], the Miller indices of the surface (hkl) must be chosen as the smallest possible integers, with the condition that $h \geq k \geq l$. A surface (hkl) may be decomposed into three microfacets each of which represents the crystallographic plane associated with the terrace, step and/or kink. One may choose any linearly independent set of three vectors for the surface normals of the microfacets, but the actual choice is arbitrary. In the following, we choose for convenience the (111) , $(11\bar{1})$ and (100) orientations to represent terraces, steps and kinks. (The choice: (111) , (110) and (100) , does not lead to significantly different results). Thus a given (hkl) surface may consist of (111) terraces, $(11\bar{1})$ steps and (100) kinks, or other suitable combinations, as will become clear below. However, it should be noted that for (hkl) values that obey the condition $h \geq k \geq l$, only (111) or (100) are possible terrace orientations.

With these choices, the ratio of the numbers of atoms associated with each of the three microfacets in an fcc surface is given by:

$$n_{(111)}:n_{(11\bar{1})}:n_{(100)} = (k+l):(k-l):(h-k) \quad (3a)$$

If the three values of $n_{(hkl)}$ obtained in this manner are ranked, the largest value, n_{\max} , will be associated with the number of terrace atoms, the middle value, n_{mid} , with the number of (non-kink) step atoms, and the smallest value, n_{\min} , with the number of kink atoms.

$$\begin{aligned} n_{\min} : n_{\text{mid}} : n_{\max} &: (n_{\min} + n_{\text{mid}} + n_{\max}) \\ &= \text{kink atoms} : \text{step atoms} : \text{terrace atoms} : \text{total atoms} \end{aligned} \quad (3b)$$

This approach leads to ambiguities whenever two of the three parameters n_{\min} , n_{mid} , and n_{\max} are equal. In the context of the present use of this approach, the ambiguity is only important with respect to identification of the terrace orientation. Whenever such an ambiguity has been present, we have used the *ad hoc* procedure of selecting the (111) orientation for the terrace as a first choice, and the (100) terrace as the second choice.

4. MODEL OF GB ENERGY

4.1 Maximum GB energy plateau

We begin by considering the energy of a GB bounded by two planes of identical hkl . We also assume that the twist angle adopts a value corresponding to the plateau region in Fig. 3a, where the energy is essentially independent of the twist angle. Thus, for the time being, we attempt to account for 4 of the 5 DoF's. The 5th DoF is addressed in Section 4.2.

The coordination number of the atoms within J planes of the two planes delimiting the GB will be higher than that at a surface but lower than that in the perfect crystal. Let us assume that the number of broken bonds of these atoms is $z_j - z'$. The GB energy may then be written as:

$$\gamma_{\text{gb}(hkl)} = \frac{2\alpha\varepsilon}{a^2} \frac{1}{\sqrt{h^2+k^2+l^2}} \sum_{i=1}^J \sum_{j=i}^J (z_j - z') \quad (4)$$

Note the factor of 2 in Eq. 4 compared with Eq. 2, which accounts for the presence of two bounding "surfaces" for the GB. If the value of the correction factor for coordination in the boundary, z' , is chosen to be proportional to z_j , Eq. 4 would lead to a constant ratio of GB energy to surface energy, a consequence which is incompatible with the results of the computer simulations (see Fig. 3c). To avoid this proportionality, we choose to modify Eq. 4 by rewriting the correction factor z' to reflect the variation in free-volume of the boundary with changes in the (hkl) of the bounding surfaces. Such an approach will break the proportionality between GB and surface energies.

In order to define a GB free-volume-like parameter, we make use of the Van Hove and Somorjai framework [15] described above. The underlying concept is that the "rougher" the two surfaces which adjoin the boundary, the larger its free-volume. In particular, it is assumed that surface roughness increases with the fraction of step and kink sites. As the fraction of these features increases, the mean spacing between steps and kinks will decrease, making it progressively more difficult for the surfaces to approach one another, especially at arbitrary values of twist angle corresponding to the GB energy plateau of Fig. 3a.

It is also necessary to include a measure of roughness for the two possible terrace orientations: (111), and (100), as the free-volumes of boundaries delimited by those surfaces will also differ somewhat from each other. The roughness of these terraces is lower for (111) and higher for (100). The effect of this terrace roughness will persist even in the case that the delimiting surfaces possess steps and kinks; however, the influence of terrace roughness should decline as the fraction of steps and kinks increases. With these considerations in mind

we formulate an expression intended to generate a term proportional to the boundary free-volume in the GB energy:

$$z_j - z'_j = [g_t(1-f_{sk}) + f_{sk}] F z_j \quad (5)$$

where g_t ($t=(111)$ or (100)) is the terrace roughness, f_{sk} is the fraction of step and kink sites, defined from Eq. 3b as: $f_{sk} = (n_{min} + n_{mid}) / (n_{min} + n_{mid} + n_{max})$, and F is a constant intended to adjust the scale of the free-volume-like expression for compatibility with the number of broken bonds in the boundary. The term, $g_t(1-f_{sk})$, is the terrace contribution to the roughness, and declines as the overall roughness of the surface, f_{sk} , increases.

The expressions for the energy of GB's with identical terminating planes, Eq. 4, may thus be rewritten with the use of Eq. 5:

$$\gamma_{gb(hkl)} = \frac{2\alpha\epsilon}{a^2} \frac{1}{\sqrt{h^2+k^2+l^2}} [g_t(1-f_{sk}) + f_{sk}] F \sum_{i=1}^J \sum_{j=i}^J z_j \quad (6)$$

In general, the term F may be viewed as an adjustable scaling factor which can be fixed by fitting to a given value of GB energy obtained either from a computer simulation or an experimental measurement.

Equation 6 is applicable to GB's bounded by two surfaces with identical (hkl) . For general GB's, bounded by the planes $(hkl)_1$ and $(hkl)_2$, the energy is written as:

$$\gamma_{gb(hkl)_1(hkl)_2}^M = [\gamma_{gb(hkl)_1} + \gamma_{gb(hkl)_2}] / 2 \quad (7)$$

where the superscript M is used to denote the maximum (plateau) GB energy (see Fig. 3a).

4.2 The 5th DoF: energy dependence on twist angle

As shown by the computer simulations [13], cusps are expected to arise in the dependence of GB energy on twist angle. These cusps occur at several possible geometric conditions. The simplest case occurs when the two planes delimiting the GB are identical, i.e. when $(hkl)_1 = (hkl)_2$. Then, at zero twist angle, both the GB and its energy vanish. At a twist angle of 180° , another deep cusp associated with a symmetric tilt boundary is obtained. Even for cases where $(hkl)_1 \neq (hkl)_2$, the computer simulations [13] show fairly deep cusps.

The approaches used thus far to define the plateau energy, do not lend themselves to a simple formulation of the cusp energies. However, since our principal purpose in developing this model is to rationalize the results of GB wetting experiments, the precise depth of the major cusps may be less important than their location in terms of twist angle, as long as the cusps are quite deep. In what follows, we therefore focus primarily on identifying the location of the cusps, and propose a rather simple approach for evaluating their depth.

In general, there are certain twist angles for which the atomic match across the GB is optimum. Consider, for example, a case where the two terminating (hkl) surfaces correspond to stepped surfaces. Then, energy cusps would be expected when the steps of one bounding surface lie parallel to the steps of the other. A similar "lock-in" concept was invoked previously by Fecht and Gleiter [16] to explain the low interfacial energies between small metal spheres and low-index orientation ionic substrates, when the close-packed rows of the metal surface fit into the valleys between the close-packed rows of the ionic crystal.

Any angular twist away from the condition of parallel steps will lead to an increase in free-volume because of step-step interference, and raise the GB energy. A twist of 180° from that orientation, where the steps are parallel once again, results in a second low energy configuration. Whereas the structures (and therefore the energies) of the two configurations need not be the same, we simplify matters in our description by assuming identical energies for

these two configurations. Furthermore, if one of the terminating GB planes corresponds to a simple terrace orientation (i.e., (111), or (100)) then additional cusps will be found in the energy as a function of twist angle, with a periodicity of π/n , where n is an appropriate symmetry factor (e.g., $n = 3$ for (111) as illustrated in Fig. 3a, and 2 for (100)). Thus, even when one of the surfaces terminating the GB corresponds to an unstepped terrace orientation, we still assume that energy minima will arise when the close packed rows of the terrace lie parallel to the steps (or close packed directions) of the other terminating plane.

We now proceed to identify the angle between the steps on the two terminating GB surfaces. Consider a GB specified by $(hkl)_1$, $(hkl)_2$ and ϕ . Let both grains (1 and 2) be referred to a common (arbitrary) reference frame in which the GB plane is defined by the normal vector \mathbf{n}_s . The directions of steps on the terminating planes of the two grains are then defined by:

$$\mathbf{k}_1 = \mathbf{t}_1 \times \mathbf{n}_s \quad \text{and} \quad \mathbf{k}_2 = \mathbf{t}_2 \times \mathbf{n}_s$$

where \mathbf{t}_1 and \mathbf{t}_2 are the normals terrace orientations of grains 1 and 2 in the reference frame. The angle ω between the steps in the plane of the GB, is given by:

$$\omega = \cos^{-1}[\mathbf{k}_1 \cdot \mathbf{k}_2]$$

With this definition, ω varies from 0 to π , and is related to the twist angle ϕ by:

$$\omega = \omega(\phi=0) + \phi, \text{ for } [\omega(\phi=0) + \phi] \leq \pi; \text{ and } \omega = 2\pi - [\omega(\phi=0) + \phi], \text{ for } [\omega(\phi=0) + \phi] \geq \pi$$

with additional periodicities for high-symmetry terminating planes, as indicated above.

Let us now consider a GB consisting of two terminating surfaces having different (hkl) , with the twist angle set at the value corresponding to $\omega = 0$, for which the GB energy is a minimum. The areal density of broken bonds of each bounding surface will in general be different. Thus, we assume that when a GB is formed from such surfaces, all the nearest neighbor bonds of the surface with the smaller broken bond density will connect to atoms of the opposite bounding surface. Thus, the minimum energy for such a boundary will depend on the absolute value of the difference between the plateau GB energies given by Eq. 6:

$$\gamma_{gb(hkl)_1(hkl)_2}^m = |[\gamma_{gb(hkl)_1} - \gamma_{gb(hkl)_2}]| \quad (8)$$

where the superscript m denotes the minimum GB energy. With this formulation, the minimum GB energy vanishes, as required, when $(hkl)_1 = (hkl)_2$. However, it also leads to zero energy for the cusp at a twist angle of 180° for cases where $(hkl)_1 = (hkl)_2$, instead of the finite energy expected for the resulting symmetric tilt boundary, and is therefore an oversimplification. We now write an expression for the GB energy of a general boundary with 5 DoF's, as:

$$\gamma_{gb(hkl)_1(hkl)_2}(\omega) = \gamma_{gb(hkl)_1(hkl)_2}^m + f(\omega) \{ \gamma_{gb(hkl)_1(hkl)_2}^M - \gamma_{gb(hkl)_1(hkl)_2}^m \} \quad (9)$$

where $f(\omega)$ is a function which can adopt values ranging from 0 at cusps, to 1 in the plateau region. In order to keep this function simple, we use the following form for $f(\omega)$:

$$f(\omega) = \sin^{0.25}(\omega) \quad (10)$$

$f(\omega)$ is intended to approximate a dependence of energy on ω which mimics a Read-Shockley form within 15° (or so) from a cusp, and adopts a constant value of unity elsewhere. More sophisticated forms for $f(\omega)$ could, of course, be used, such as for example, a Fourier series which produces any desired shape for the twist angle dependence. However, given the simplicity of the model, a more complex representation does not appear to be warranted.

5. MODEL PREDICTIONS AND COMPARISON WITH EXPERIMENTAL RESULTS

5.1 Qualitative trends of the model

For the purpose of these comparisons, we simplify matters by assigning values of unity to both F and ε/a^2 . The parameters $g_{(111)}$ and $g_{(100)}$ were optimized so as to yield minimum scatter (i.e. maximum R-value) in a linear plot of the plateau GB energy versus mean surface energy. The plot is shown in Fig. 6a for the optimized values: $g_{(111)} = 0.47$ and $g_{(100)} = 0.62$. This shows that the trends obtained from the model are generally consistent with the results of the simulations (cf Fig. 1c) in that the GB energy is roughly a linear function of mean surface energy and that it extrapolates to zero GB energy at a finite value of surface energy. Thus, while the constants g_i may be viewed as adjustable parameters, they have been fixed here, once and for all, to provide qualitative agreement with the trends observed in computer simulations. These values should therefore apply to the GB's of any fcc material.

We also compare in Fig. 6b the dependence of GB energy computed by means of the model on the assumed GB free volume parameter. For a general GB this may be defined by:

$$\bar{V} = \{ \{g_i(1-f_{sk})+f_{sk}\}(hkl)_1 + \{g_i(1-f_{sk})+f_{sk}\}(hkl)_2 \} F / 2 \quad (11)$$

where the subscript i in $(hkl)_i$ signifies evaluation of the expression for the i th (hkl) . Figure 6b shows the desired linear relationship, with the best line passing close to the origin. Thus the characteristics of the model for the maximum GB energies, corresponding to the plateau region of Fig. 3a, are generally similar to those of the simulations.

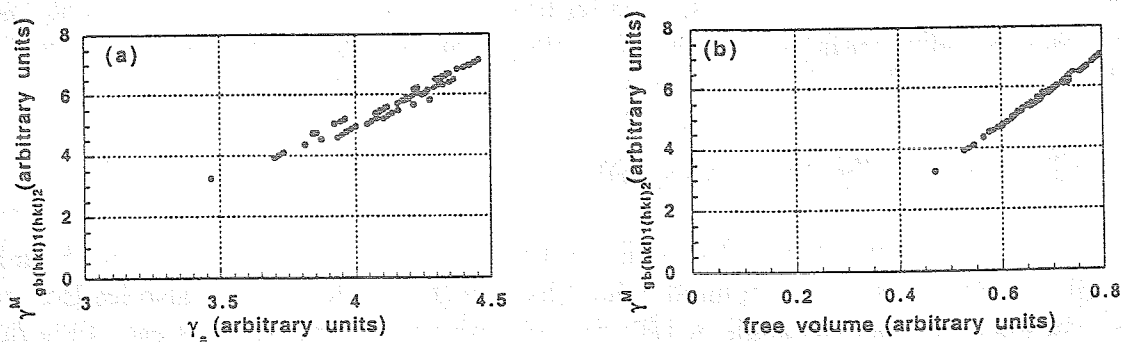


Figure 6. Plots of the plateau GB energies, computed by means of Eq. 12, (a) vs. the mean surface energy, and (b) vs. the free-volume parameter defined in Eq. 11, for all possible combinations of bounding planes given in Fig. 1.

5.2 Comparison with GB Wetting Results

We now proceed to a more rigorous test of the model by comparing its predictions against the experimental results on GB wetting. GB wetting should prevail when:

$$\gamma_{gb}(hkl)_1(hkl)_2(\omega) / [\gamma_{sl}(hkl)_1 + \gamma_{sl}(hkl)_2] \geq 1 \quad (12)$$

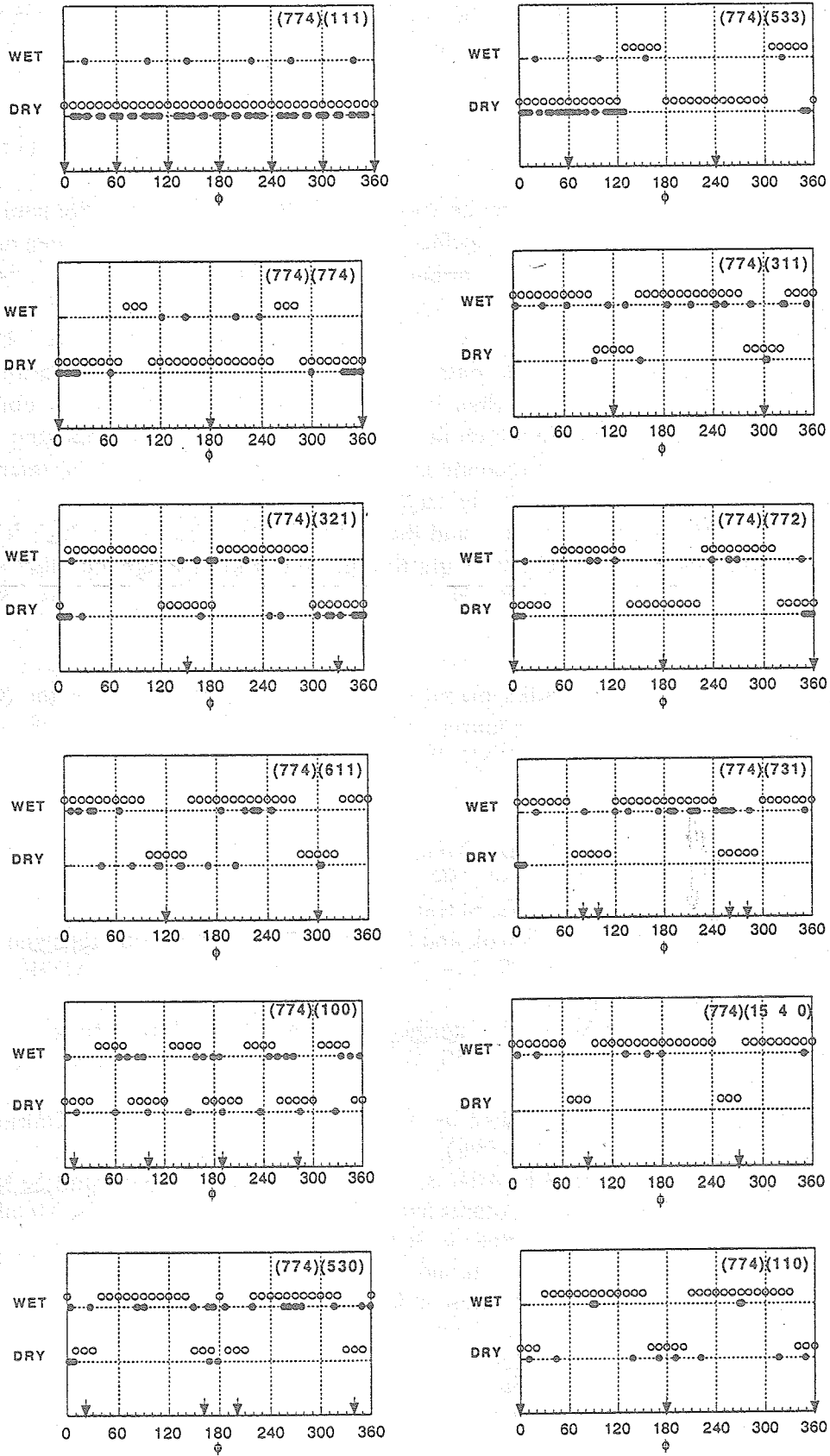


Figure 7. Comparison between GB wetting data (filled symbols) and model predictions (open symbols) for the 12 cases of GB's terminated by a (774) surface on one side. The arrows indicate the locations where steps on the terminating surfaces are parallel.

where $\gamma_{sl(hkl)_i}$ ($i=1,2$) are the energies of the solid-liquid interfaces formed when liquid contacts each of the two GB terminating surfaces. Each of these interfaces may be considered to consist of a surface in contact with a disordered array of liquid atoms, where the number of broken bonds is lower than that at a free surface by a factor FG . Thus:

$$\gamma_{sl(hkl)_i} = FG \gamma_{s(hkl)_i} \quad (13)$$

where $\gamma_{s(hkl)_i}$ is given by Eq. 2, and G may be viewed as an additional adjustable parameter for relating solid-liquid interfacial energy to surface energy. Since F has already been assigned a value of unity, G is the only adjustable parameter used in the following comparisons with wetting data, and is assigned a value of 0.58. Comparisons are shown in Fig. 7 for a subset of the data consisting of all GB's terminated by (774) surfaces on one side, and all other surfaces shown in Fig. 1 on the other side. The data represent more than 300 observations of GB wetting. Agreement with predictions has been quantified by accepting as correct any experimental point with a twist angle which falls within $\pm 5^\circ$ of a correct prediction. This is a reasonable range over which to test agreement in view of the estimated 10° experimental error. Correct predictions are found in over 80% of cases.

Given the simplicity of the model, and the rather simple manner in which it accounts for cusp energy, this degree of agreement is gratifying. To our knowledge, no other analytical models are presently available to calculate GB energy as a function of all 5 macroscopic DoF's.

Acknowledgments.

The authors acknowledge with thanks primary support of this research by the MERSEC program of the National Science Foundation under grant DMR9632556. PW also wishes to acknowledge NSF support under grant DMR9802290.

References

1. B.L. Adams, S.I. Wright, and K. Kunze, *Metall. Trans. A24*, 819 (1993).
2. B.L. Adams, *Mater. Sci. Eng. A166*, 59 (1993).
3. M. Weins, H. Gleiter and B. Chalmers, *Scripta Met.* 4, 235 (1970).
4. G.H. Bishop, Jr., R.J. Harrison, T. Kwok and S. Yip, in Interatomic Potentials and Crystalline Defects, edited by J.K. Lee (The Metallurgical Society of AIME, Warrendale, PA, 1981), p.357
5. D. Wolf and K. L. Merkle, in Materials Interfaces -- Atomic Level Structure and Properties, edited by D Wolf and S. Yip (Chapman and Hall, New York, N.Y., 1990), p.87.
6. V. Vitek, in Stability of Materials, edited by A. Gonis, P.E.A. Turchi and J. Kudrnovsky (Plenum Press, New York N.Y. 1996), p.53
7. M. Takashima, P. Wynblatt and B.L. Adams, in Grain Growth in Polycrystalline Materials III, edited by H. Weiland, B.L. Adams and A.D. Rollett, (The Minerals, Metals & Materials Society, Pittsburgh, 1998) p. 365.
8. M. Takashima, A.D. Rollett, P. Wynblatt and B.L. Adams, in Proceedings of ICOTOM-12, edited by J.A. Szpunar (NRC Research Press, 1999) p.1649.
9. M. Takashima, P. Wynblatt and B.L. Adams, *Interface Sci.*, to be published.
10. D. Wolf and J.F. Lutsko, *Z. Kristallogr.* 189, 239 (1989).
11. D. Wolf, *Acta Metall.* 37, 1983 (1989).
12. D. Wolf, *Acta Metall.* 37, 2823 (1989).
13. D. Wolf, *Acta Metall. Mater.* 38, 791(1990).
14. Y.W. Lee and H.I. Aaronson, *Acta Metall.* 28, 539 (1980); *Surf. Sci.* 95, 227 (1980).
15. M.A. Van Hove and G.A. Somorjai, *Surf. Sci.* 92, 489 (1980).
16. H.J. Fecht and H. Gleiter, *Acta Metall.* 33, 557 (1985).