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Never ending saga of a simple boundary

Dedicated to Professor Dr. Dr. h. c. Manfred Rühle on the occasion of his 65th birthday

The structure and associated translational states of the $\Sigma = 3(112)$ symmetrical tilt grain boundary in niobium and molybdenum are investigated theoretically by three distinct computational methods. The results are compared with those of previous theoretical studies as well as with transmission electron microscopy observations. It was found that for this grain boundary, when fully relaxed, two possible translation states – "reflection" and "sheared" – are energetically almost degenerate in the two transition metals studied and thus comparison with experiments is ambivalent. This prevents the $\Sigma = 3(112)$ boundary from being a suitable benchmark for validations of semi-empirical theoretical models of interatomic interactions.

Keywords: Body-centered cubic metals; Grain boundaries; Computer modeling; Ab-initio and semi-empirical schemes

1. Introduction

Grain boundaries are the most common and most important interfaces in crystalline materials since they control a broad variety of physical and mechanical properties. This is the reason why they have been studied very extensively throughout the development of materials science. In general, grain boundaries may not possess any periodicities. However, boundaries with periodic structures have frequently been observed and, at least in cubic materials, any grain boundary may be approximated as closely as desired by a boundary with a periodic structure. Such periodic boundaries can be fully characterized and geometrically constructed using the concept of the coincidence site lattice (CSL), first introduced by Brandon et al. [1]. While the basic attributes of periodic boundaries are crystallographic [1–6], it is their atomic structure that is of principal importance and the main object of research. This structure differs very significantly from that of the bulk in a narrow region, usually spanning only several lattice spacings, and all the significant interfacial phenomena occur in this region.

Crystallographically, a grain boundary is fully characterized by the relative misorientation of the adjoining grains, orientation of the corresponding rotation axis, orientation of the boundary plane, and in the case of lattices with basis, position of the boundary plane; this represents six independent parameters. However, these parameters do not determine uniquely the atomic structure of grain boundaries and both atomistic modeling [7–11] and experimental observations [10, 12–16] revealed structural multiplicity of crystallographically well-defined boundaries. In most cases, multiple structures correspond to different relative translations of the adjoining grains. Such translations represent three more degrees of freedom but these are determined by minimization of the boundary energy when the six chosen crystallographic parameter shave been fixed. In some cases the multiple structures are related bya symmetry operation of the bicrystal and in this case they are energetically degenerate [12]. However, more commonly, they possess different energies and it is then the lowest energy structure which is expected to be found. The ground state of a grainboundary is in this case uniquely associated with the corresponding relative displacement of the grains.

Investigation of the relative translation of the grains provides an opportunity to link atomistic studies of grain boundaries with observations using transmission electron microscopy. Earlier studies, that employed the α-fringe method, indeed confirmed the existence of relative displacements of the adjoining grains away from the coincidence site lattice positions and corroborated the results of atomistic studies of several grain boundaries inaluminum [12, 17]. More recently, the high-resolution transmission electron microscopy (HRTEM) has been employed in such investigations [16, 18–22]. An important goal of the studies of translation states of grain boundaries is to test the applicability of descriptions of interatomic interactions employed in atomistic calculations, assuming that the translation state is uniquely determined by the minimization of the boundary energy [22–24].

The boundary, the translation state of which has been studied since early seventies, is the $\Sigma = 3(112)$ boundary in body-centered cubic (bcc) metals, which is the symmetrical tilt grain boundary (STGB) associated with deformation twins in this crystal structure. The initial calculations [25–27] were carried out using Johnson's empirical pair potential for iron [28] and oscillatory pair potentials for simple metals [29]. Latter calculations employed ad-band tight-binding scheme for transition metals [30]. More recently this boundary was investigated in several bcc transition metals [31] employing the many-body central force potentials of the Finnis–Sinclair type [32, 33] together with potentials based on the tight-binding method that include the scalar fourth and matrix second moments of the density of states [34, 35]. A general result of all these calculations is that there are two possible translation states of this boundary.

In the first case, there is no relative displacement of the two grains away from the exact coincidence site positions and the mirror symmetry across the boundary plane ispreserved. This, so-called "eflection" structure, is shown in Fig. 1a. In the second case, the upper grain is displaced with respect to the lower grain parallel to the boundary plane by the vector $t = 1/12[11\bar{1}]$. The corresponding structure, shown in Fig. 1b, is called "sheared" or "isosceles" structure [26]. It no longer possesses the mirror symmetry with respect to the boundary plane but not all symmetry is lost in this structure. A two-fold screw axis (shown as the horizontal line in Fig. 1b) exists along the direction located midway between the last (112) plane of the bottom grain and the first (112) plane of the displaced upper grain.

In the calculations employing Johnson's pair potential [25–27] and oscillatory pair potentials [29], the sheared structure was found to possess marginally lower energy than the reflection structure while the opposite was found in the tight-binding calculations of Papon et al. [30]. In the calculations of Marinopoulos et al. [31] the reflection structure was found as the only stable one when using Finnis–Sinclair central-force potentials for VIA-group transition metals Mo and W (the sheared structure corresponds to a maximum rather than minimum energy configuration with respect to relative displacement of the grains), while the sheared structure was the most stable one for VA-group element Nb. On the other hand, in the same study, when using the Carlsson's potentials for Mo and W that include directional bonding, both structures were found to be metastable and the sheared structure was found to be favored, albeit marginally. Thus, previous calculations do not provide a clear cut answer which of the two structures is the low energy one and whether there exists a common preference for a particular translation state in bcc metals in generalor whether and how the grain boundary structure differs from metal to metal.

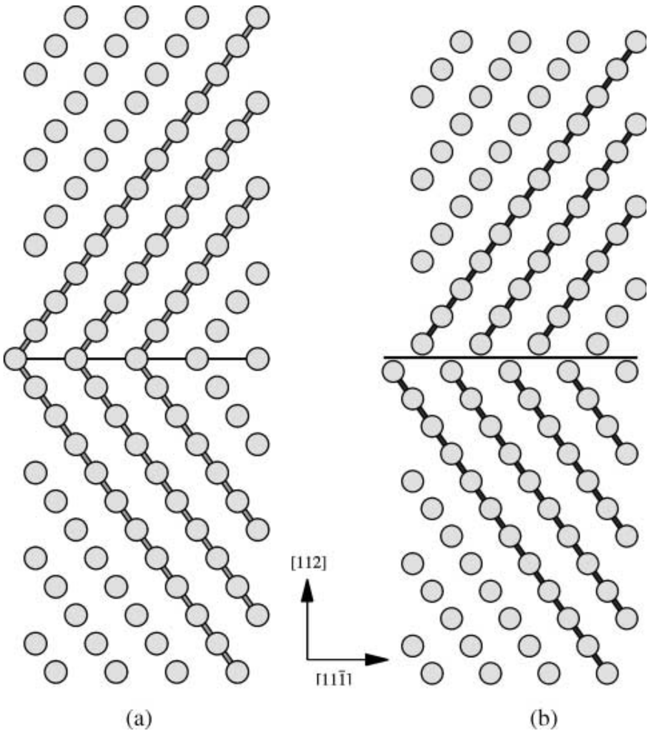

Fig. 1. Schematic picture of the reflection (a) and sheared (b) structures of the $\Sigma = 3$ (112) twin grain boundary in the $[1\bar{1}0]$ projection.

Surprisingly, a similar situation appears in transmission electron microscopy studies. The reflection structure was found in α-iron [36] and Fe-3 %Si [37]. On the other hand, two recent HRTEM observations in molybdenum arriveat different results. Vystavel et al. [16] conclude that only the sheared structure exists while observations of Tsurekawa et al. [38] are inconclusive and suggest that both structures may exist. While it is entirely possible that structures with different translation states will occur in different bcc metals, it is natural to expect that a specific structure will be favored ina given material.

In the present paper, we address the question of translation states at the $\Sigma = 3(112)$ boundary in molybdenum and niobium by carrying out the atomistic calculations of this boundary using the *ab initio*, density functional theory based, mixed-basis pseudopotential method [39–42], the environment-dependent orthogonal tight-binding model [43] and the recently constructed screened bond order potentials [44]. Comparison of the three sets of calculations also provides an assessment of the accuracy of the semi-empirical potentials. The results of the three approaches suggest a near degeneracy of the two translation states implying that comparison of observed and calculated displacement states of this boundary cannot serve as a test of the quality of semi-empirical descriptions of interatomic interactions.

2. Computational approaches

Three distinct computational approaches that include explicitly the electronic structure were used for the investigation of the atomic structure of the $\Sigma = 3$ (112) STGB in molybdenum and niobium.

First, the *ab initio* mixed-basis pseudopotential (MBPP) method was employed as a benchmark calculation. This method is based on the density functional theory [45, 46] with the local density approximation for exchange and correlation [47, 48]. Its accuracy and reliability have been confirmed in several previous studies for abroad range of materials. One of the preceeding applications of this approach, directly related to the current study, was the investigation of the $\Sigma = 5$ (310) STGB in bcc transition metals by Ochset al. [23, 24]. The relevant computational details described there are the same as in the present study and we will not repeat them here.

Second, the semi-empirical environment-dependent tight-binding (EDTB) model developed by Haas et al. for Mo [43, 49] and parameterized by Haas for Nb [50] (cf. Ref. [51], Appendix A) was utilized. This method employs a minimal basis set of atomic orbitals to represent s-, p- and d-valence electron interactions. The Hamiltonian matrix elements and the repulsive potential terms are environmentally dependent to enhance the transferability of the scheme. The method uses standard k-space procedures to solve for the total energy and forces and thus requires supercells with periodic boundary conditions.

Third, the screened bond order potentials (SBOP) [44] with environment-dependent bond integrals [52] were employed. The SBOP scheme is based on real-space parameterized tight-binding model in which diagonalization of the Hamiltonian is substituted by direct evaluation of the bond order via the Green's functions formalism using the recursion scheme with nine moments of the local density of states [53–56]. Furthermore, this improved version of bond order potentials implicitly accounts for non-orthogonality effects via the analytic environmental dependence of bond integrals. The advantage of the real-space formalism in SBOP scheme is that it eliminates the need for three-dimensional periodic boundary conditions and thus adds more-flexibility to calculations of extended defects.

It is important to emphasize that since both the EDTB and SBOP methods are based on quantum mechanical principles, they are able to describe correctly directional bonds arising due to the d-electrons which is crucial for a correct description of the energetics in bcc transition metals. However, both approaches are at the same time semi-empirical which means that these models are fitted to a finite set of *ab initio* and/or experimental data for specific atomic configurations. Hence, there is no *a priori* guarantee that such parameterization is fully transferable to other configurations. However, since both these methods were employed successfully in the extensive comparative study of the $\Sigma = 5$ (310) boundary [23], we anticipate that they provide adequately reliable results for the $\Sigma = 3$ (112) grain boundary.

The calculations of total energies and atomic forces were done with supercells containing 24 atoms with full periodic boundary conditions. These supercells are comprised of two grains of the bcc metal in the $\Sigma = 3$ twin misorientation and contain two $\Sigma = 3$ (112) grain boundaries, about 5 lattice spacings apart. The geometry andorientation of the ideal reflection supercell is displayed in Fig. 2.

In order to achieve a complete and consistent comparison of results, both *ab initio* MBPP and semi-empirical EDTB and SBOP calculations were carried out with the same 24-atom supercell even though all three methods are able to handle larger block sizes and SBOP does not require the periodic boundary conditions. Extensive tests were carried out with EDTB using 18-atom to 30-atom supercells [51], and with SBOP using larger simulation cells without imposing periodic boundary conditions perpendicular to the interface plane [44], to ensure that the 24-atom supercells are large enough and the two equivalent interfaces sufficiently far separated to avoid undesirable influences on the investigated stability of boundaries with different translation states.

3. Results and discussion

The possible translation states of the $\Sigma = 3(112)$ STGB were investigated by calculating the variation of the total energy as a function of relative displacements of the two grains in the supercell. The procedure is analogous to that employed in the studies of the $\Sigma = 5$ (310) STGB [23, 24] and follows the general method of γ-surfaces used for exploring the metastable planar faults (see e. g. Refs. [57, 58]).

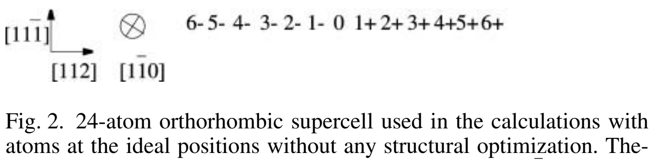

Fig. 2. 24-atom orthorhombic supercell used in the calculations with atoms at the ideal positions without any structural optimization. The-large and small circles correspond to atoms at different $(1\bar{1}0)$ planes.

In the fully relaxed configurations the axial translations, i. e., grain displacements along the [112] direction that lead to expansion and/or contraction perpendicular to the boundary plane, were found tobe marginal, less than 0.1 Å for both Nb and Mo, with all three approaches. This agrees with the previous findings of the detailed atomistic simulations for Mo by Marinopoulos et al. [31]. Experimentally, a considerably larger axial translation of 0.3 Å, derived from a quantitative HRTEM image analysis, was reported in [16]. In the same work, atomistic simulations carried out by Pontikis [59] were cited, which yielded axial translations of only 0.1 Å, supporting both the findings of Marinopoulos et al. [31] and our results. In a subsequent paper of the same group [15] the axial translation in the same bicrystal of Mo was investigated using the α-fringe technique in transmission electron microscopy. The very small value of the axial translation (0.05 ± 0.02 Å) found using this technique agrees with the findings of the atomistic simulations. Very recently, the twin bicrystal was re-examined by HRTEM using a microscope with correction for the three-fold astigmatism [60]. The axial translation was again found to be smaller than 0.1 Å, consistent with the value of Ref. [15] and the theoretical values. Hence, the axial excess expansion at the $\Sigma = 3$ (112) boundary is very small, less then 0.1 Å, and, therefore, it may be expected to have only a minor influence on interface structure and properties. Apparently, the large expansion reported in Ref. [16] originated from the uncorrected three-fold astigmatism of the microscope used.

Considering lateral grain displacements along the $[\bar{1}10]$ direction, parallel to the tilt axis, energy minima were obtained at zero displacements for all three computational approaches and both metals studied. Hence, the $(\bar{1}10)$ planes of both grains areal ways aligned. This is in full agreement with the experimental observation in Ref. [16] as well as with the previous atomistic simulations [25–28, 30, 31, 59].

The lateral grain displacements of primary interest are those along the $[11\bar{1}]$ direction, perpendicular to the tilt axis. As mentioned in the introduction, two high-symmetry configurations corresponding to different relative displacements of the grains exist, the reflection state with the mirror symmetry and the sheared state with the two-fold screw-rotation symmetry (see Fig. 1). These are the most likely metastable translation states though other possibilities are not precluded. The calculated dependencies of the energy versus displacement for niobium and molybdenum are displayed in Figs. 3a and b, respectively. In these figures the sheared structure corresponds to zero displacement and is marked as (S), while the reflection structure corresponds to the displacements $\pm 0.144\,a$, where a is the lattice spacing, and is marked as (R). The reason for placing the origin of displacements at thesheared configuration is explained below.

The curves in Figs. 3a and b represent the variation of the energy for rigid relative displacements of the grains without any additional relaxation. The full symbols mark the energies of the two high-symmetry translation states with all atomic positions in the supercells relaxed to zero forces. In the case of rigid displacements the energy attains a stationary (minimum or maximum) value dictated by the symmetry only for the sheared configuration. However, when all

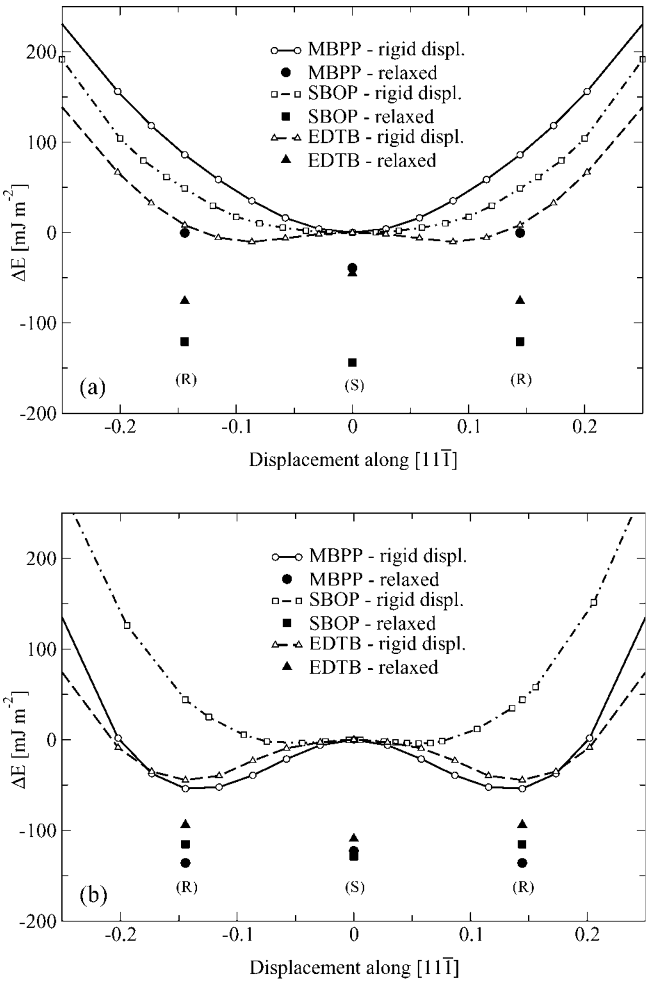

Fig. 3. Energy of the $\Sigma = 3$ (112) grain boundary vs lateral displacement of the grains along the [$11\bar{1}$] direction, measured in units of the lattice parameter a. Zero displacement corresponds to the sheared structure, marked (S); (R) denotes the reflexion structure (see text for explanation of this placement of the origin). The curves correspond to rigid relative displacements of the grains without any relaxation and the full symbols to fully relaxed sheared and reflexion structures. The energy is measured relative to the unrelaxed sheared structure. (a) Niobium; (b) molybdenum.

the atoms are fully relaxed, both the sheared and the reflection states are stationary owing to the symmetry. This subtle aspect of the symmetry is linked with the position of the central atomic layer of the supercell (marked as 0 in Fig. 2) relative to the neighboring layers in the two grains. For the rigid displacement it is attached to one side, while by relaxation it adjusts its position such that the shifts along [$11\bar{1}$] and [$\bar{1}\bar{1}1$]become equivalent. Because of this peculiarity only the sheared structure is associated with an energy extremum in both unrelaxed and relaxed situations and, consequently, in order to attain the closest possible comparison for the energy versus displacement dependencies from all three methods, it is advantageous to choose the origin of the displacement axes in Fig. 3 at the sheared structure. Eventhough choosing the reflection structure as the undisplaced state may appear to be a more "natural" choice since it corresponds to the CSL configuration, it would cause the three curves to cross each other and obscure the differences in their shapes.

As seen from Fig. 3a, for Nb the sheared configuration corresponds to the only minimum energy with respect to the rigid displacements of the grains in calculations employing MBPP. When all atoms are fully relaxed both the sheared and reflection structures are metastable but the sheared structure remains favored over there flection structure by about 40 mJ m^{-2}. The SBOP gives qualitatively the same result as the MBPP, only the difference between energies of fully relaxed sheared and reflection structures is smaller. On the other hand the EDTB indicates that the sheared structure is unstable for rigid displacements and a shallow energy minimum emerges about half way between the sheared and the reflection displacement states. By relaxation the position of this minimum shifts and the fully-relaxed structure coincides with the reflection configuration. The sheared configuration remains metastable after relaxation with energy which is 31 mJ m^{-2} higher than that of the relaxed reflection structure. Thus, for Nb the SBOP results mimic closely those of the MBPP while the EDTB calculations fail to do so. Nevertheless, since to our knowledge no experimental observations of the displacement state of the $\Sigma = 3$ (112) in Nb have been reported, the MBPP prediction itself awaits an experimental validation.

In the case of Mo the situation is opposite to that of Nb in calculations employing MBPP. As seen from Fig. 3b, for the rigid displacements of the grains the sheared configuration corresponds to a maximum of energy and an energy minimum is found very close to the reflection state. After full relaxation both the sheared and reflection structures are again found to be metastable, but as mall energetic preference of 13 mJ m^{-2} for the reflection structure remains. For rigid displacements the EDTB results follow closely those of MBPP both qualitatively and quantitatively. However, after full relaxation the sheared structure becomes energetically favored by 16 mJ m^{-2} over the reflection structure. In the case of SBOP and rigid grain displacements the sheared structure is marginally unstable and a very shallow minimum, corresponding to the displacement of $0.06\,a$, emerges. However, after full relaxation the situation is very similar to that found using EDTB. Both the sheared and reflection structures are metastable and the sheared structure is favored by 10 mJ m^{-2} over the reflection structure. Hence, in the prediction of the ground state structure both EDTB and SBOP contradict the MBPP prediction, although the differences of corresponding energies are only of the order of 10 mJ m^{-2}, which represents less than 2 % of the grain boundary energy.

For Mo, two experimental observations of translation states of the $\Sigma = 3$ (112) STGB are available for comparison with calculations. Vystavel et al. [16] derive from their HRTEM analysis that the observed state is the sheared one, while Tsurekawa et al. [38] provide some evidence for the presence of both displacement states in different regions of the boundary. Thus, even experimental observations do not clearly answer the question about the translation state of the $\Sigma = 3$ (112) STGB in Mo.

The calculated energies of the two fully relaxed structures of the $\Sigma = 3$ (112) STGB, as well as energy differences between the two competing structures, are summarized for both Nb and Mo in Table 1. A common result of all three methods employed in this paper is that the energy differences between the two competing structures corresponding to distinct translation states are very small. The *ab initio* MBPP calculations yield little but still significant energetic preference for the reflection structure in the case

Table 1. The first two columns show the energy differences between the reflection and sheared structures in the case of rigid grain displacements and fully relaxed structures, respectively. The last two columns summarize the energies of the fully relaxed sheared and reflection structures. All energy values are in mJ m^{-2}.

		Niobium		
Method	$\Delta E^{\text{unrelaxed}}_{\text{R-S}}$	$\Delta E^{\text{relaxed}}_{\text{R-S}}$	E_S	E_R
MBPP	+84	+40	255	295
CPMD	+74	–	–	–
SBOP	+49	+20	517	540
EDTB	+8	-31	218	187
		Molybdenum		
MBPP	−54	−13	463	450
CPMD	−77	–	–	–
SBOP	+44	+10	786	796
EDTB	-45	+16	416	432

MBPP: mixed-basis pseudopotential method
CPMD: Car-Parinello molecular dynamics
SBOP: screened bond order potentials
EDTB: environment-dependent tight binding

of Mo and the sheared structure in the case of Nb. The predictive power of *ab initio* density-functional methods for small structural energy differences is well established. Nevertheless, a few cases are known in which disparities with experimental observations were reported that were attributed to the local density approximation or to generalized gradient corrections. However, for Nb and Mo both the local density approximation and generalized gradient corrections have been very successful [40, 61, 62]. Furthermore, in the case of the rigid displacements the energy differences between the reflection and sheared structures found by MBPP were very closely reproduced for both Mo and Nb by independent *ab initio* calculations of Meyer employing the Car-Parrinello molecular-dynamics (CPMD) method [63]. Therefore, we believe that the predicted ground states of the $\Sigma = 3$ (112) STGB are, indeed, the lowestenergy states at 0 K in pure Nb and Mo.

Notwithstanding, for Mo the result of MBPP calculations is obviously in disagreement with the experimental observations of Vystavel et al. [16], while the experimental observations in Ref. [38] are indecisive. At the same time, the results of EDTB and SBOP calculations, which predict that the sheared structure is favored, agree with Ref. [16]. However, this does not imply that the approximate tight-binding based methods are better capable to predict the correct structure than the *ab initio* calculations. The predicted energy differences between the two competing structures with distinct translations are so small that they require a very high numerical accuracy of the computational approach involved. For *ab initio* calculations such a numerical accuracy can, indeed, be achieved with sufficient computational effort, while for the two semi-empirical approaches such precision is likely at or beyond their limits since their correctness is constrained by various physical and computational approximations inherent in these schemes. Since both the reflection and sheared structures are metastable and differ only marginally in energy, it is possible that both occur under different experimental conditions. In both experiments [16, 38], noticeable deviations from the ideal twin misorientation were present and such non-ideal misorientations, as well as other local structural imperfections of the bicrystals, may affect the translation state when the energy differences are very small. Thus the agreement between experiments in Ref. [16] and calculations that employed EDTB and SBOP has to be regarded as fortuitous. Nevertheless, the calculations demonstrate that for the fully relaxed structures these approximate schemes lead to virtually the same results as the *ab initio* MBPP calculations within the achievable precision.

4. Conclusions

The $\Sigma = 3$ (112) STGB in bcc transition metals was expected to provide a suitable model system for validation of the reliability of theoretical models for description of interatomic interactions. For a simple grain boundary, such as this one, it is possible to obtain information about its atomic structure and, in particular about the relative translations of the grains, from experimental HRTEM observations as well as from the state-of-the-art *ab initio* calculations. Thus, it is possible, at least in principle, to achieve a detailed quantitative comparison of calculations and experiments. However, the results of this study lead to the conclusion that this model boundary is not at this stage of experimental and theoretical capabilities suitable for this purpose. The reasons are the following: Theoretically, certain physical and computational approximations inherent to the computational approaches impose limits on the reliability and predictive power when the energy differences between different structures are below a certain limit. In the case of the $\Sigma = 3$ (112) twin this limit is apparently reached for the tight-binding based methods EDTB and BOP though not necessarily for the *ab initio* MBPP method. At the same time, small tilt or twist deviations away from the desired ideal twin misorientation of the bicrystals, accompanied by interfacial dislocations, and/or spurious amounts of segregated impurities, can never be avoided in real high-quality transmission electron microscopy specimens. It is then possible that such small deviations from the ideal structures may be associated with energy differences comparable to those found in the calculations of energies of alternate structures and may thus stabilize either one of the energetically almost degenerate configurations with different translations. Therefore, unlike the $\Sigma = 5$ (310) STGB [22, 23], the $\Sigma = 3$ (112) STGB appears less promising as a benchmark for experimental validations of semi-empirical theoretical models of interatomic interactions since it is much more demanding on the precision in both experiments and calculations.

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