# Supplemental material: Modeling of Deformation Twinning in BCC Metals via Quantum Annealing

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December 4, 2025

## 1 Interfacial Energy

From a pure continuum elasticity perspective, the elastic energy presents a four fold symmetry, which is presented in the polar plots in Figure 2 of the main manuscript. However, from a crystallographic perspective, the 90° rotation would lead to a $(\bar{1}\bar{1}1)$ boundary which is not a twin interface, in agreement with common knowledge of deformation twinning in bcc metals. Obviously continuum elasticity is not aware of this atomic scale effect. This is not a deficit of the continuum description, which is intended to capture the behavior beyond atomic scales, but rather supports the necessity to penalize improper non-twin boundaries by a higher interfacial energy for capturing the correct crystallographic aspect. Therefore, an interfacial energy contribution is needed to give preference to the expected twin interface.

We use a simple approach for modeling the interfacial energy between domains. At these boundaries, we have a different spin value on both sides of the interface. Therefore, the approach is to use an additional energy contribution

$$H_s = \sum_{i<j} J_{ij} s_i s_j + H_0 = \sum_{i<j,\text{n.n.}} \sigma(\theta) A_{ij} \frac{s_i s_j - 1}{2}$$

with only quadratic interaction terms, with $\sigma(\theta)$ denoting an orientation dependent interaction energy and $A_{ij}$ as area of the common interface between the domains. In the simplest case, only nearest neighbor interactions (n.n.) in horizontal ($\sigma(\theta = \pi) = \sigma_|$) and vertical direction ($\sigma(\theta = 0) = \sigma_-$) are considered, see Figure S1. We note that a horizontal nearest neighbor spin pair of different orientation corresponds to vertical interface, hence the subscript of the interfacial energy $\sigma$ indicates the corresponding interface orientation. On the domain discretization level, inclined interfaces consist of steps (see Figure S1), which allows to calculate the effective macroscopic interfacial energy in large systems. In the case of equal values $\sigma_| = \sigma_-$, the energy for horizontal and vertical interfaces coincide, but the angular dependence shows a weak anisotropy, see left panel of Figure S2. Choosing $\sigma_-$ and $\sigma_|$ differently allows to suppress the non-twin grain boundaries with $(\bar{1}\bar{1}1)$ orientation, see Figure S2 (center) for a case with $\sigma_| = 2\sigma_-$. Here, a vertical interface, which is assumed to coincide with the crystallographically undesired orientation, becomes unfavorable. For the present simulations, we use this formulation of the anisotropic interfacial energy to exemplarily demonstrate the suppression of the undesired grain boundary and splitting of twins into smaller lamellae.

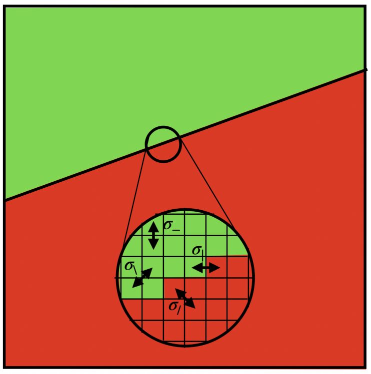

**Figure S1:** Sketch of the representation of interfaces through nearest neighbor interactions on the domain scale.

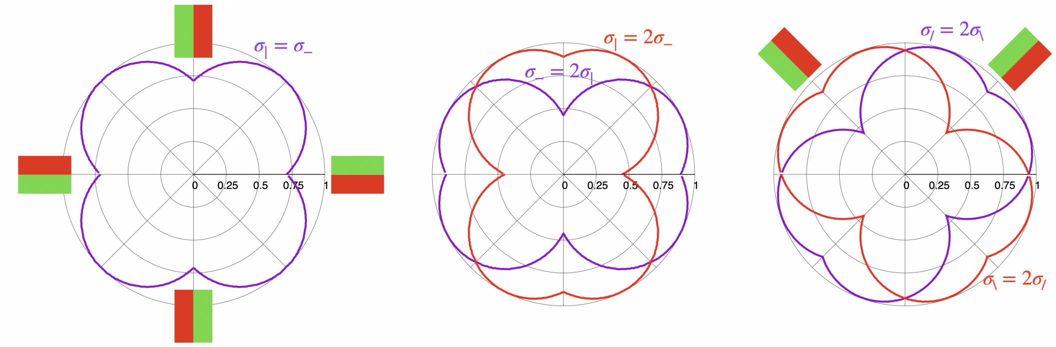

**Figure S2:** Orientation dependent interfacial energy. Left panel: Only horizontal and vertical nearest neighbor interactions are used, with equal magnitude ($\sigma_- = \sigma_|$). Center: The two values are chosen differently to enhance the anisotropy of the grain boundary energy, with the intention to suppress the crystallographically undesired ($\bar{1}\bar{1}1$) interface orientation and the favor (112) twin boundaries. Right panel: Here, only diagonal nearest neighbor interactions are used, to reflect the interfacial energy anisotropy of crystals which are rotated by $\pm\pi/4$. In each figure, the values are scaled to the maximum value. The pictures illustrate the interface orientations in the polar plots.

For polycrystalline simulations, where also the lattice orientations are rotated, the interfacial energy needs to be adjusted. The simplest case of a 90° rotation is reflected through the choice $\sigma_{-} = 2\sigma_{|}$ (Figure S2 center). For a rotation by $\pi/4$ we need to involve diagonal nearest neighbor interactions, $\sigma_{/}$ and $\sigma_{\backslash}$. In comparison to $\sigma_{-}$ and $\sigma_{|}$ they need to be re-normalized by $1/\sqrt{2}$ to account for the "staircase representation" of a tilted interface, and the increased number of diagonal interactions, to be equivalent to the non-rotated crystal (Figure S2 right panel). For arbitrary grain orientations we use here for simplicity the interfacial energy representation of one of the cases discussed above, which is closest in orientation. We note that more accurate expressions for the interfacial energy are possible and will be discussed separately.