

Phase-field model study of the effect of interface anisotropy on the crystal morphological evolution of cubic metals

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Abstract

An expression is proposed for the anisotropy of interfacial energy of cubic metals, based on the symmetry of the crystal structure. The associated coefficients can be determined experimentally or assessed using computational methods. Calculations demonstrate an average relative error of <3% in comparison with the embedded-atom data for face-centred cubic metals. For body-centred-cubic metals, the errors are around 7% due to discrepancies at the {332} and {433} planes. The coefficients for the {100}, {110}, {111} and {210} planes are well behaved and can be used to simulate the consequences of interfacial anisotropy. The results have been applied in three-dimensional phase-field modelling of the evolution of crystal shapes, and the outcomes have been compared favourably with equilibrium shapes expected from Wulff's theorem.

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1. Introduction

Crystals are by their very nature anisotropic and interfaces between crystals similarly have energies and structures that are orientation dependent. Phase-field models used to simulate microstructural development have attempted to incorporate this interfacial anisotropy in a variety of ways. The free energy density for a heterogeneous system with contributions from the chemical free energy and interface energy is represented by:

$$g(\varphi, c, T) = g_0(\varphi, c, T) + \frac{1}{2} \varepsilon^2 |\nabla \varphi|^2, \quad (1)$$

where g is the system free energy density, g_0 is the chemical free energy density, φ is phase-field order parameter, c is solute concentration, T is temperature and ε is the gradient energy coefficient. Interfacial anisotropy is generally introduced by making ε orientation-dependent. For example, in

the two-dimensional simulation of cubic crystals it is common to assume that [1]:

$$\varepsilon = \bar{\varepsilon} [1 + \gamma_\varepsilon \cos(k_\varepsilon \theta)], \quad (2)$$

where $\bar{\varepsilon}$ is the mean value of ε , θ is the polar angular coordinate of the interface normal, and γ_ε and k_ε are anisotropy parameters. Eq. (2) has been modified into other formats to fulfil specific simulation targets [2,3]. In three-dimensional phase-field models, the Cahn–Hoffman ξ vector theory has been applied to describe the interface anisotropy [4,5]. A suggestion made by Karma and Rappel for cubic crystals is [6]:

$$\varepsilon = \bar{\varepsilon} \left[1 + \gamma_\varepsilon (n_x^4 + n_y^4 + n_z^4) \right], \quad (3)$$

where n_x , n_y and n_z are Cartesian coordinates of the interface normal. More recently, Haxhimali et al. suggested that the gradient energy coefficient takes the following format to represent interface anisotropy in the context of phase fields [7]:

$$\varepsilon = \bar{\varepsilon} [1 + \varepsilon_1 K_1(\theta, \Phi) + \varepsilon_2 K_2(\theta, \Phi) + \dots], \quad (4)$$

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where θ and Φ represent the orientation of the interface in spherical coordinates, ε_1 and ε_2 are coefficients reflecting the extents of anisotropy, K_1 and K_2 are cubic harmonics that are combinations of standard spherical harmonics with cubic symmetry. The addition of the $\varepsilon_2 K_2$ term in Eq. (4) (cf. Eq. (3)) is a result of reviewing molecular dynamics simulations for dendrite growth which suggest that this gives a better representation of anisotropy [8].

The motivation for the present work was to develop a generic expression for interface anisotropy of cubic metals, to specify coefficients in the resulting expression and to validate the concept against existing knowledge of crystal growth.

2. Interface energy anisotropy

In a cubic system, the normal to a plane with Miller indices (hkl) plane is the direction [hkl]. The unit normal \hat{n} has Cartesian coordinates n_x , n_y and n_z . Fig. 1 illustrates how these can be represented in polar or spherical coordinates:

$$n_x = \sin \theta \cos \phi = \frac{h}{\sqrt{h^2 + k^2 + l^2}} \quad (5.1)$$

$$n_y = \sin \theta \sin \phi = \frac{k}{\sqrt{h^2 + k^2 + l^2}} \quad (5.2)$$

$$n_z = \cos \theta = \frac{l}{\sqrt{h^2 + k^2 + l^2}}. \quad (5.3)$$

Anisotropy energy, in general, can be represented as expansions of n_x , n_y and n_z in various orders. In discussing magnetocrystalline anisotropy [9], the interface anisotropy is represented by:

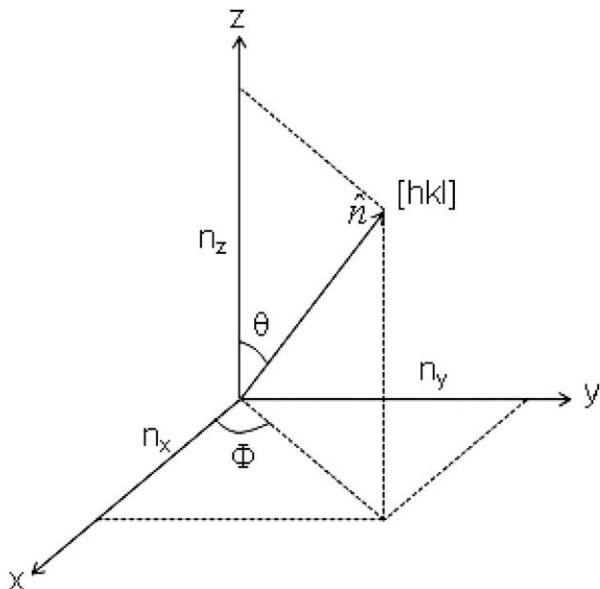


Fig. 1. Relation between Miller indices, and Cartesian and polar coordinates in a cubic system.

$$\sigma(\hat{n}) = k_0 + \sum_{i,j} k_1 n_i n_j + \sum_{i,j,u,w} k_2 n_i n_j n_u n_w + \dots, \quad (6)$$

where k_0 , k_1 , k_2 and k_3 are the defining coefficients. The subscripts of n represent the Cartesian coordinates. For cubic symmetry, this simplifies into [10]:

$$\sigma(\hat{n}) = k_0 + k_1 (n_x^2 n_y^2 + n_y^2 n_z^2 + n_z^2 n_x^2) + k_2 n_x^2 n_y^2 n_z^2 + k_3 (n_x^2 n_y^2 + n_y^2 n_z^2 + n_z^2 n_x^2)^2 + \dots \quad (7)$$

Ignoring the higher-order terms and using Miller indices, Eqs. (5) and (7) give:

$$\sigma(h, k, l) = k_0 + k_1 \frac{h^2 k^2 + k^2 l^2 + l^2 h^2}{(h^2 + k^2 + l^2)^2} + k_2 \frac{h^2 k^2 l^2}{(h^2 + k^2 + l^2)^3} + k_3 \frac{(h^2 k^2 + k^2 l^2 + l^2 h^2)^2}{(h^2 + k^2 + l^2)^4}. \quad (8)$$

For given anisotropy coefficients k_0 , k_1 , k_2 and k_3 , Eq. (8) can express the interfacial energy as a function of orientation.

Eq. (8) is different from the expansion based on cubic harmonics [6,7] – for example, the leading anisotropic term in Eq. (7) is not $(n_x^4 + n_y^4 + n_z^4)$ but $(n_x^2 n_y^2 + n_y^2 n_z^2 + n_z^2 n_x^2)$. Critical assessment of those two different expressions for representing crystal anisotropy is important but is beyond the scope of the present work. However, it is obvious that Eq. (8) is consistent with cubic symmetry. For example, the interfacial energy for all directions of the form $\langle 100 \rangle$ is k_0 . For $\langle 110 \rangle$ it is $k_0 + k_1 + k_3$, for $\langle 111 \rangle$ it is $k_0 + k_1/3 + k_2/9 + k_3/9$, etc. So, in conclusion, although the individual coefficients cannot be identified with symmetry elements the equation as a whole is consistent with cubic symmetry.

It is required to validate the description inherent in Eq. (8) for cubic anisotropy. The method here was fitted to results from the embedded-atom method (EAM) [11,12]. These EAM calculations are based on embedding atomic functions and electronic densities given by Baskes et al. [13–15]. The least-squares method was used to fit the data with the following objective function:

$$\delta = \sum_i [\sigma(h, k, l) - \sigma_{EAM}(h, k, l)]^2, \quad (9)$$

where i is the total number of EAM data, $\sigma(h, k, l)$ is from Eq. (8) and $\sigma_{EAM}(h, k, l)$ from EAM data. The best values of k_0 , k_1 , k_2 and k_3 are obtained when δ achieves a minimum, i.e. at $\partial \delta / \partial k_j = 0$ with $j = 0, 1, 2$ and 3 . Fig. 2 demonstrates the efficacy of Eq. (8) for 10 face-centred cubic (fcc) crystals, and the corresponding derived values of anisotropy coefficients together with the average relative errors (AvRE) are listed in Table 1. AvRE is defined as $AvRE = \frac{|\sigma(h, k, l) - \sigma_{EAM}(h, k, l)|}{\sigma_{EAM}(h, k, l)}$. It can be seen that 9 out of 10 fits have $< 2\%$ average relative errors.

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