Nucleation of Grain Boundary Phases: Supplemental Materials

I. S. Winter,[1, *] R. E. Rudd,[1] T. Oppelstrup,[1] and T. Frolov[1, †]

[1] *Lawrence Livermore National Laboratory, Livermore, California 94550, USA*

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QUASI-2D MODEL OF HOMOGENEOUS GRAIN BOUNDARY PHASE NUCLEATION

To begin the treatment of the quasi-2D nucleation theory, two phases: β (the parent phase) and α (the new phase) are defined as shown in Fig. 1 and the actual structure of the respective phases is shown in Fig. 3. The difference in grain boundary energy as a result of the nucleation of a new phase is written as $\Delta\gamma^{\alpha\beta} = \gamma^\alpha - \gamma^\beta$. The length of the α phase nucleus is defined as l. As Fig. 1 infers the presence of the α nucleus within the β phase creates both a dislocation and a line force (due to the difference in grain boundary stress) at the interface of the two phases, which will both generate an elastic field of their own. The change in energy per unit length as a result of the nucleation of the α phase can be expressed as

$$\frac{E^{2D}}{L} = \Delta\gamma^{\alpha\beta}l + \frac{E^{dd}}{L}(l) + \frac{E^{pp}}{L}(l) + \frac{E^{dp}}{L}(l) + 2\Gamma^{\alpha\beta}, \tag{1}$$

where $\frac{E^{dd}}{L}(l)$ is the elastic interaction energy between the two dislocations generated by the formation of the α phase, $\frac{E^{pp}}{L}(l)$ is the elastic interaction energy of the two line forces, $\frac{E^{dp}}{L}(l)$ is the interaction between the dislocation and line force and $\Gamma^{\alpha\beta}$ is the energy per unit length of the grain boundary phase junction: it is not a function of nucleus size for this 2D example. It should be noted that $\Gamma^{\alpha\beta}$ implicitly includes the core energies of the two dislocations created by the grain boundary phase junction, which does not include the energy of the elastic field.

The elastic interaction between the two dislocations generated from the nucleation process can be expressed as [1]

$$\frac{E^{dd}}{L}(l) = -\frac{\mu}{2\pi}\left[(\boldsymbol{b}^1 \cdot \boldsymbol{\xi})(\boldsymbol{b}^2 \cdot \boldsymbol{\xi}) + \frac{(\boldsymbol{b}^1 \times \boldsymbol{\xi}) \cdot (\boldsymbol{b}^2 \times \boldsymbol{\xi})}{1-\nu}\right]\ln(l/\rho) \\ -\frac{\mu}{2\pi(1-\nu)l^2}\left[(\boldsymbol{b}^1 \times \boldsymbol{\xi}) \cdot \boldsymbol{l}\right]\left[(\boldsymbol{b}^2 \times \boldsymbol{\xi}) \cdot \boldsymbol{l}\right], \tag{2}$$

where $\boldsymbol{b}^1$ and $\boldsymbol{b}^2$ represent the Burgers vectors of the two dislocations, $\boldsymbol{\xi}$ the dislocation line direction, μ the shear modulus of the bulk material, ρ the dislocation core radius (and is assumed to be b), and ν Poisson's ratio. For the purposes of this work we will assume that the dislocation generated at the phase junction is a general mixed dislocation: $\boldsymbol{b}^1 = b_1\hat{\boldsymbol{e}}_1 + b_2\hat{\boldsymbol{e}}_2 + b_3\hat{\boldsymbol{e}}_3$, $\boldsymbol{b}^2 = -b_1\hat{\boldsymbol{e}}_1 - b_2\hat{\boldsymbol{e}}_2 - b_3\hat{\boldsymbol{e}}_3$, $\boldsymbol{l} = l\hat{\boldsymbol{e}}_1$ and $\boldsymbol{\xi} = 1\hat{\boldsymbol{e}}_2$. As there is no Burgers
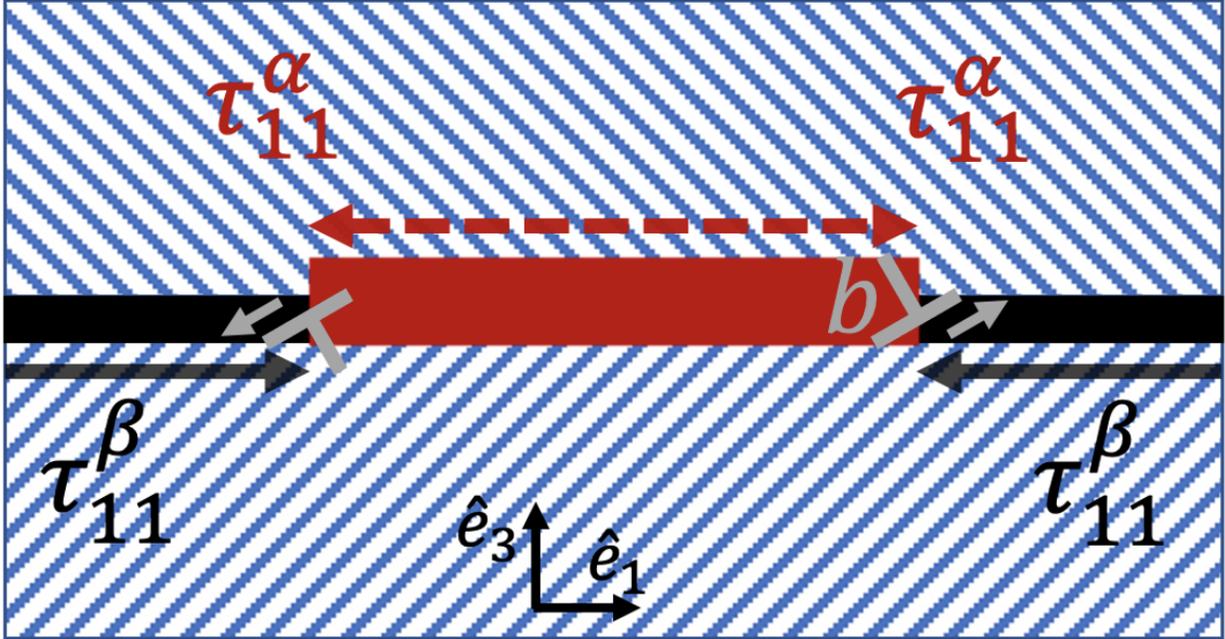
FIG. 1. Illustration of the important interactions to consider in the homogeneous nucleation of the α grain boundary phase (red region). It should be noted that $\hat{e}_2$ is going into the page. Apart from the difference in grain boundary energy between the two phases, there are also elastic interactions that arise from the presence of dislocations (due to geometric constraints) and line forces (due to differences in grain boundary stress) at the phase boundaries.

content in the grain boundary before the nucleation of the new grain boundary phase it must be true that $\boldsymbol{b}^1 + \boldsymbol{b}^2 = 0$, due to the conservation of Burgers vectors. In the case of a general mixed dislocation Eq. (2) simplifies to

$$\frac{E^{dd}}{L}(l) = \frac{\mu}{2\pi}\left(b_2^2 + \frac{(b^e)^2}{1-\nu}\right)\ln\left(l/\rho\right) + C^{dd} \tag{3}$$

with $b^e = \sqrt{b_1^2 + b_3^2}$ being the edge component of the dislocation and b_2 being the screw component, and C^{dd} being the remaining terms which are not dependent on l.

A line force will exist at the boundary between the two phases of the form $f_1 = \pm(\tau_{11}^\alpha - \tau_{11}^\beta)$, with the sign changing depending on if the left $(-)$ or right $(+)$ phase junction shown in Fig. 1 is considered. The displacement field associated with the line force is found using the following expression [2]

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$$u_i(\boldsymbol{x}) = \int G_{ij}^{PS}(\boldsymbol{x} - \boldsymbol{x}')f_j\delta(x_1 - x_1')\delta(x_3 - x_3')d\boldsymbol{x}', \tag{4}$$

with all subscripts pertaining to a 2D space ($i \in \{1, 3\}$), $\boldsymbol{x} = x_1\hat{\boldsymbol{e}}_1 + x_3\hat{\boldsymbol{e}}_3$, δ being Dirac's Delta function and G_{ij}^{PS} being the elastic Green's function of an isotropic medium for a plane stress problem, which is expressed as [2]

$$G_{ij}^{PS}(\boldsymbol{x}) = \frac{1}{8\pi\mu(1-\nu)}\left(\frac{x_i x_j}{x^2} - (3 - 4\nu)\delta_{ij}\ln(x)\right). \tag{5}$$

As the elastic interaction between two line forces, in general, is given by $-f_j^{(1)}u_j^{(2)}(l\hat{\boldsymbol{e}}_1)$, the interaction in this case should be of the form

$$\frac{E^{pp}}{L} = f_i f_j G_{ij}^{PS}(l\hat{\boldsymbol{e}}_1). \tag{6}$$

In this case $f_1 = \tau_{11}^\alpha - \tau_{11}^\beta$. By combining Eqs. (4-6) E^{pp} is found to be

$$\frac{E^{pp}}{L}(l) = -\frac{f_1^2(3 - 4\nu)}{8\pi\mu(1-\nu)}\ln(l/\rho) + C^{pp}, \tag{7}$$

with C^{pp} representing all terms that are not dependent on l.

Finally, the elastic interaction between the dislocation and force-monopole will be considered. The elastic interaction of a dislocation with a line force is given by

$$\frac{E^{dp}}{L} = -2f_1 u_1^{dis}(l\hat{\boldsymbol{e}}_1). \tag{8}$$

with $\boldsymbol{u}^{dis}$ being the displacement field of the dislocation located a length l away from the line force. The displacement field of an edge dislocation is given by[1]

$$(u^{dis})_1' = \frac{b^e}{2\pi}\left[\tan^{-1}\left(\frac{x_3'}{x_1'}\right) + \frac{x_1' x_3'}{2(1-\nu)(x_1'^2 + x_3'^2)}\right], \tag{9a}$$

$$(u^{dis})_3' = -\frac{b^e}{2\pi}\left[\frac{1 - 2\nu}{4(1-\nu)}\ln\left(x_1'^2 + x_3'^2\right) + \frac{x_1'^2 - x_3'^2}{4(1-\nu)(x_1'^2 + x_3'^2)}\right], \tag{9b}$$

where $x_1' = x_1\cos(\phi) + x_3\sin(\phi)$ and $x_3' = -x_1\sin(\phi) + x_3\cos(\phi)$, with ϕ being the angle that makes the expression for the edge components of the dislocation $\boldsymbol{b}^e = b^e\cos(\phi)\hat{\boldsymbol{e}}_1 + b^e\sin(\phi)\hat{\boldsymbol{e}}_3$ true. Combining equations (8) and (9) results in

$$\frac{E^{dp}}{L} = -\frac{f_1 b_3(1 - 2\nu)}{2\pi(1-\nu)}\ln(l/\rho) + C^{dp} \tag{10}$$

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Combining the three elastic interaction terms together with the difference in grain boundary energy between the two phases, the energy of the system with a nucleus is given by

$$
\frac{E^{2D}}{L} = \Delta\gamma^{\alpha\beta}l + \frac{1}{8\pi(1-\nu)}\left(4\mu\left[(1-\nu)b_2^2 + (b^e)^2\right] - \frac{(f_1^\alpha - f_1^\beta)^2(3-4\nu)}{\mu}\right.
$$
$$
\left. - 4(f_1^\alpha - f_1^\beta)b_3(1-2\nu)\right)\ln(l/\rho) + 2\Gamma^{\alpha\beta} + C. \tag{11}
$$

For $\Delta\gamma^{\alpha\beta} < 0$, E decreases for large l and increases for small. A maximum at l^c represents the nucleation barrier. The size of the critical nucleus is determined by solving $\frac{dE^{nuc}(l)}{dl} = 0$ for l, which gives

$$
l^c = \frac{4\left[(1-\nu)b_2^2 + (b^e)^2\right]\mu^2 - 4\mu b_3 f_1(1-2\nu) - f_1^2(3-4\nu)}{8\pi\mu\Delta\gamma^{\alpha\beta}(\nu-1)}. \tag{12}
$$

Using molecular dynamics simulations in combination with Eq. (11) we can calculate $\Gamma^{\alpha\beta}$. The simulations consist of constructing a grain boundary phase nucleus (α) within an existing grain boundary phase (β) and then calculating the change in grain boundary energy as a function of the nucleus length. $\Gamma^{\alpha\beta}$ is calculated by finding the value of $\Gamma^{\alpha\beta}$ that gives a best fit between Eq. (11) and the results of the molecular dynamics simulations.

The grain boundary phase junction was created by first generating a bicrystal with a kink of height $3a_0/2$ along the grain boundary. The dual-phase system was constructed by displacing the top crystal relative to the lower crystal by $\boldsymbol{t}^1 = 1.704\text{Å}\hat{\boldsymbol{e}}_1 + 2.057\text{Å}\hat{\boldsymbol{e}}_2$, as shown in Fig. 2a: $\boldsymbol{t}^1$ corresponds to a displacement that will give the β phase upon relaxation. Then a region of the upper crystal, of length l along the $\hat{\boldsymbol{e}}_1$-direction, was further displaced by $\boldsymbol{t}^2 = 0.852\text{Å}\hat{\boldsymbol{e}}_1$. The combination of shifts, $\boldsymbol{t}^1 + \boldsymbol{t}^2$, should result in the formation of the α phase in the given region upon relaxation. The combined system is then relaxed such that the maximum force between atoms was 10^{-5} eV/Å, with the resulting final dual-phase system illustrated in Fig. 2b.

3D MODEL OF HOMOGENEOUS GRAIN BOUNDARY PHASE NUCLEATION

A three-dimensional model of homogeneous grain boundary phase nucleation is developed for a circular grain boundary phase nucleus with a radius, R. The equation governing the
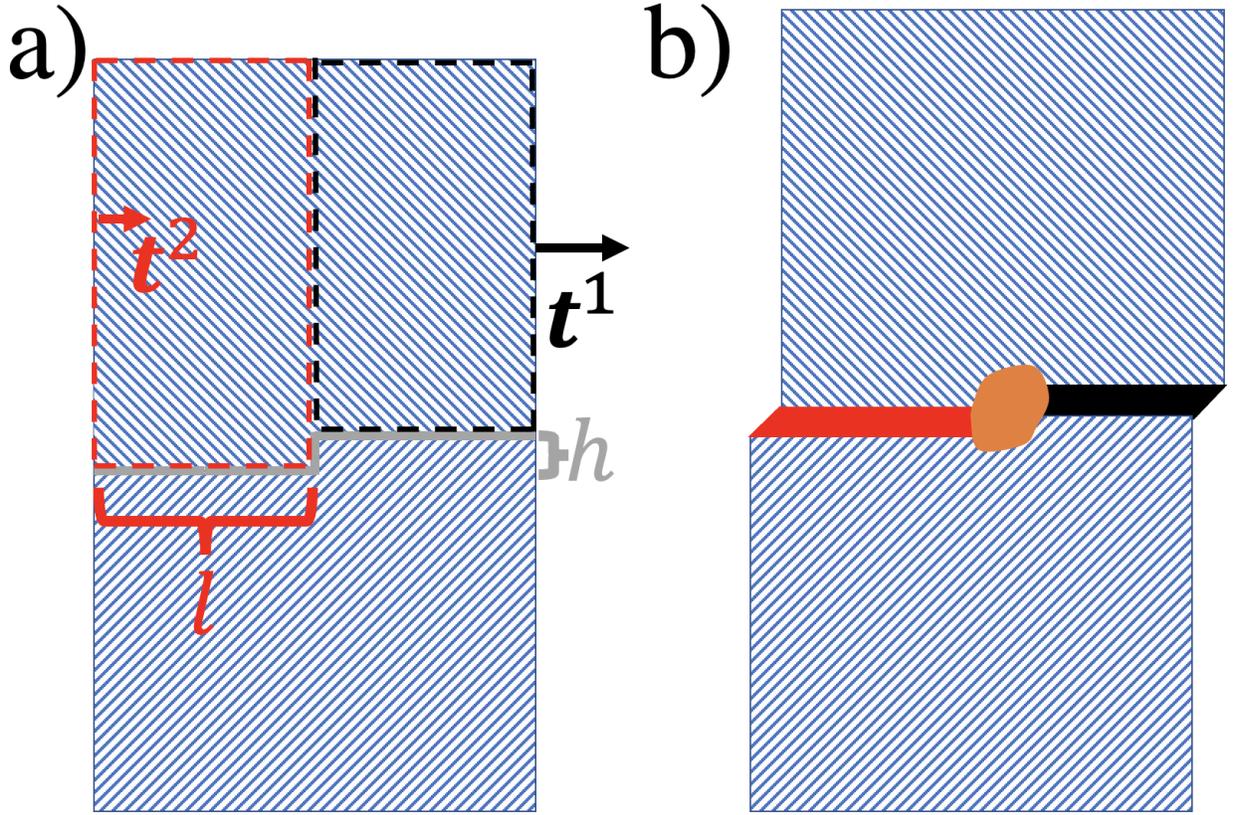
FIG. 2. Illustration of the setup of the molecular dynamics simulations used to validate the classical nucleation theory. Panel a depicts two crystals, separated by an interface with a kink of height h, being displaced relative to each other. By displacing a section of the upper crystal of length l by $\boldsymbol{t}^2$ and the rest of the upper crystal by the vector $\boldsymbol{t}^1$ as shown in Panel a, a dual phase grain boundary is created after relaxing the system, as shown in Panel b. The core of the grain boundary junction is signified by the orange region.

nucleation energy will be of the form

$$E^{nuc}(R) = \pi R^2 \Delta \gamma^{\alpha\beta} + 2\pi R \bar{\Gamma}^{\alpha\beta} + E^{dd}(R) + E^{dp}(R) + E^{pp}(R). \tag{13}$$

The derivation of the elastic terms, $E^{dd}(R) + E^{dp}(R) + E^{pp}(R)$, as well as the line energy term, $2\pi R \bar{\Gamma}^{\alpha\beta}$, follow. We assume in the 3D model that the grain boundary phase junction is circular, and thus the dislocation associated with it is a dislocation loop. The self-energy of a dislocation loop is expressed as [1]
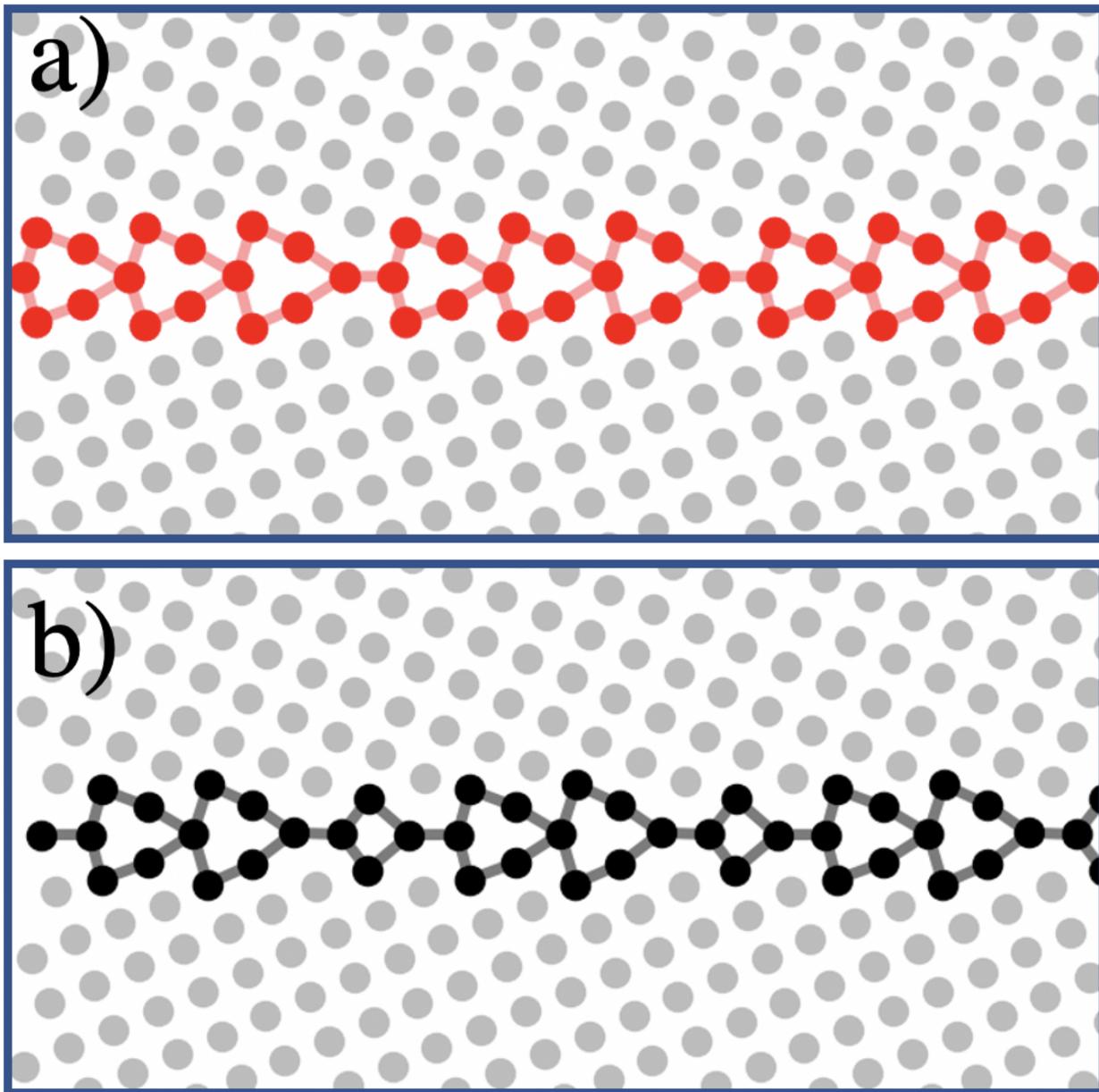
FIG. 3. Panel a shows the α phase (ground state) and panel b shows the β phase (metastable).

$$E^{dd} = \frac{\mu}{8\pi} \oint_{C_1=C} \oint_{C_2=C} \frac{(\boldsymbol{b} \cdot d\boldsymbol{\xi}^1)(\boldsymbol{b} \cdot d\boldsymbol{\xi}^2)}{r} + \frac{\mu}{8\pi(1-\nu)} \oint_{C_1=C} \oint_{C_2=C} (\boldsymbol{b} \times d\boldsymbol{\xi}^1) \cdot \boldsymbol{T} \cdot (\boldsymbol{b} \times d\boldsymbol{\xi}^2), \quad (14)$$

where $T_{ij} = \frac{1}{r} \left(\delta_{ij} - \frac{r_i r_j}{r^2} \right)$ and the rest of the variables are defined in Fig. 4. The line integral shown in Eq. (14) will produce an infinite energy if evaluated as is, due to the self-interaction of a differential segment with itself. Thus, a core radius must be defined to allow for a finite self-energy. This approximation turns Eq. (14) into
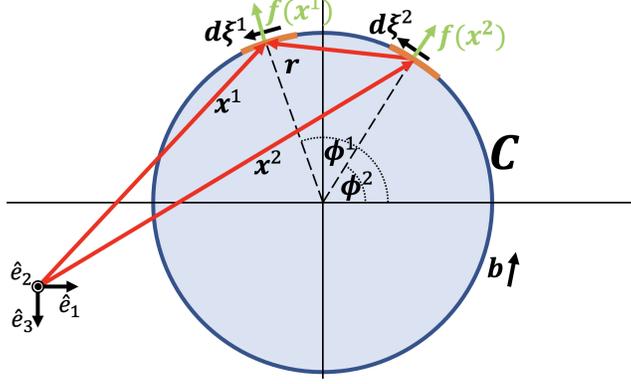
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FIG. 4. Graphical representation of a grain boundary phase nucleus and variables involved in Eq. (14), (17), and (21), with $\boldsymbol{C}$ defining the contour of the grain boundary phase junction.

$$E^{dd}(R) = \frac{\mu R^2}{8\pi} \int_0^{2\pi} \int_{\phi_2+\rho/R}^{\phi_2+2\pi-\rho/R} \frac{[\boldsymbol{b} \cdot d\boldsymbol{\xi}^1(\phi_1,\phi_2)][\boldsymbol{b} \cdot d\boldsymbol{\xi}^2(\phi_1,\phi_2)]}{r(\phi_1,\phi_2)} d\phi_1 d\phi_2$$
$$+ \frac{\mu R^2}{8\pi} \int_0^{2\pi} \int_{\phi_2+\rho/R}^{\phi_2+2\pi-\rho/R} \frac{[\boldsymbol{b} \times d\boldsymbol{\xi}^1(\phi_1,\phi_2)] \cdot \boldsymbol{T}(\phi_1,\phi_2) \cdot [\boldsymbol{b} \times d\boldsymbol{\xi}^2(\phi_1,\phi_2)]}{1-\nu} d\phi_1 d\phi_2.$$
(15)

Evaluation of this integral for the system in question results in

$$E^{dd}(R) = \frac{\mu R}{4(1-\nu)} \left[\left(2b_3^2 + (b^p)^2(2-\nu)\right) \ln\left(\frac{4R}{\rho}\right) - 2\left(b_3^2 + (b^p)^2(2-\nu)\right) \right], \qquad (16)$$

with $(b^p)^2 = b_1^2 + b_2^2$. ρ is the core radius of the dislocation, and is assumed to be of the magnitude b.

For the line force-line force interaction, the following equation gives the elastic self-energy of a line force loop

$$E^{pp}(R) = - \oint_{C_1=C} \oint_{C_2=C} f_j(\boldsymbol{x}^1) G_{jk}(\boldsymbol{x}^1 - \boldsymbol{x}^2) f_k(\boldsymbol{x}^2) d\boldsymbol{x}^1 d\boldsymbol{x}^2, \qquad (17)$$

with $\boldsymbol{G}$ being the three-dimensional elastic Green's function for an isotropic system, and defined as

$$G_{ij}(\boldsymbol{x}) = \frac{1}{16\pi\mu(1-\nu)} \left(\frac{(3-4\nu)}{x} \delta_{ij} + \frac{x_i x_j}{x^3} \right). \qquad (18)$$

Using the same approach for evaluating the line integral of the dislocation-dislocation interaction, the line integral in Eq. (17) becomes

$$E^{pp}(R) = -f_j f_k \int_0^{2\pi} \int_{\phi_2+\rho/R}^{\phi_2+2\pi-\rho/R} G_{jk}(\phi_1, \phi_2) d\phi_1 d\phi_2. \tag{19}$$

Taking into account that in the case of the circular line force loop, $\boldsymbol{f} = f_1 \cos\phi \hat{\boldsymbol{e}}_1 + f_2 \sin\phi \hat{\boldsymbol{e}}_3$ meaning that by using the same approach to solve Eq. (17) as that used to determine Eq. (15) the line force self-energy is expressed as

$$E^{pp}(R) = -\frac{R}{32\mu(1-\nu)} \left[\left(f^2(13-16\nu) - 2f_1 f_2 \right) \ln(4R/\rho) - 4f^2(7-8\nu) \right], \tag{20}$$

where $f^2 = f_1^2 + f_2^2$. It should be noted that $f_2 = (\tau_{22}^\alpha - \tau_{22}^\beta)$.

Lastly, $E^{dp}(R)$ can be expressed as

$$E^{dp}(R) = -2 \oint_C f_j(\boldsymbol{x}) u_j^{dis}(\boldsymbol{x}) d\boldsymbol{x}, \tag{21}$$

where u_j^{dis} is the displacement field of the circular dislocation loop. The displacement field of the circular dislocation loop is expressed as [1]

$$u_m^{dis}(\boldsymbol{x}) = -\frac{1}{8\pi} \oint_C \epsilon_{mik} \frac{2b_i}{r} dx_k' - \frac{1}{8\pi(1-\nu)} \oint_C b_i \epsilon_{ijk} T_{mj} dx_k', \tag{22}$$

with $\boldsymbol{\epsilon}$ being the Levi-Civita tensor. By combining eqs. (21) and (22) the interaction energy is found to be

$$E^{dp}(R) = -\frac{(f_1 + f_2)b_3 R}{2(1-\nu)} \left((1-2\nu)\ln(4R/\rho) - 3 + 4\nu \right). \tag{23}$$

As $\Gamma^{\alpha\beta}$ contains the dislocation core energy of the grain boundary junction, it is reasonable to assume that it depends on the Burgers vector and dislocation line direction. The contribution of the line energy to the nucleation energy of a 3D system requires an effective value of the line energy:

$$\bar{\Gamma}^{\alpha\beta} = \frac{1}{2\pi} \int_0^{2\pi} \Gamma^{\alpha\beta}(\boldsymbol{b}, \boldsymbol{\xi}(\phi)) d\phi, \tag{24}$$

with the dislocation line direction, $\boldsymbol{\xi}$, being a function of ϕ, specifically $\boldsymbol{\xi} = -\sin\phi \hat{\boldsymbol{e}}_1 + \cos\phi \hat{\boldsymbol{e}}_2$. For a better understanding of the dependence of $\boldsymbol{\xi}$, Fig. 4 can be of help.

In developing a functional form for $\Gamma^{\alpha\beta}(\phi)$ it is helpful to note that axes of symmetry exist along the $\hat{\boldsymbol{e}}_1$ and $\hat{\boldsymbol{e}}_3$ directions in the form of a two-fold rotation and mirror plane normal

respectively [3]. Applying these two symmetries to $\Gamma^{\alpha\beta}$ mean that the grain boundary phase junction energy must be an even function with respect to ϕ, $\Gamma^{\alpha\beta}(\phi) = \Gamma^{\alpha\beta}(-\phi)$.

Assuming that the function is continuous and differentiable it also means that $\Gamma^{\alpha\beta}(\phi = 0)$ and $\Gamma^{\alpha\beta}(\phi = \pi)$ must be local extrema. Owing to the fact that the $\Gamma^{\alpha\beta}$ is calculated from molecular dynamics simulations, which use a dislocation dipole configuration to derive the core energy of the phase junction, we cannot differentiate between $\Gamma^{\alpha\beta}(\phi = 0)$ and $\Gamma^{\alpha\beta}(\phi = \pi)$, thus we approximate that they are equal.

If $\Gamma^{\alpha\beta}(0)$ and $\Gamma^{\alpha\beta}(\pi)$ are local minima (maxima), there must be a local maximum (minimum) along the domain $\phi \in (0, \pi)$. We postulate that the other local maximum (minimum) is situated at $\phi = \pi/2$ and $\phi = 3\pi/2$. It is found that $\Gamma^{\alpha\beta}(0) = \Gamma^{\alpha\beta}_{min} = 0.383$ eV/Å and $\Gamma^{\alpha\beta}(\pi/2) = \Gamma^{\alpha\beta}_{max} = 1.73$ eV/Å. A function that fits the above requirements is

$$\Gamma^{\alpha\beta}(\phi) = \frac{\Gamma^{\alpha\beta}_{max} - \Gamma^{\alpha\beta}_{min}}{2} [1 - \cos(2\phi)] + \Gamma^{\alpha\beta}_{min}. \tag{25}$$

Combining Eqs. 24 and 25 results in the line energy contribution to be $2\pi R \frac{\left(\Gamma^{\alpha\beta}_{max} + \Gamma^{\alpha\beta}_{min}\right)}{2}$.

COMPUTATIONAL DETAILS OF MOLECULAR STATICS AND DYNAMICS SIMULATIONS

The setup for the simulations used to validate the 3D CNT are similar to those used to validate the quasi-2D CNT, with the exception being that instead of creating a rectangular region containing the nucleating grain boundary phase, the nucleating phase exists in a circular region of the grain boundary defined by a radius, R. The dimensions of the system are $100\sqrt{29}a_0 \times 500a_0 \times 6\sqrt{29}a_0$ with the system being periodic in the $\hat{e}_1$ and $\hat{e}_2$ directions. Like in Fig. 2, the grain boundary phase junction is created by first generating a bicrystal that only contains the β phase, which is obtained by displacing the top crystal relative to the lower crystal by $\boldsymbol{t} = 1.704\text{Å}\hat{e}_1 + 2.057\text{Å}\hat{e}_2$, then a cylindrical region is defined that runs through the entire upper crystal with its axis pointed along the $\hat{e}_2$ direction and which has a radius of R. This cylindrical region is then shifted relative to the rest of the upper crystal by $\boldsymbol{t} = 0.852\text{Å}\hat{e}_1$. The resulting structure contains approximately 17.5 million atoms, thus a full structural relaxation is exceedingly difficult to achieve. As a result, the structure was relaxed by running the structure at 1000 K for 1.25 ns, and then quenching the structure from 1000 K to 0 K over the course of 0.5 ns.

DSC LATTICE

In order to determine the admissible disconnections that can exist at a grain boundary the displacement shift complete (DSC) lattice must be known, as disconnections are lattice vectors on the DSC lattice. All points on the DSC lattice can be described by a linear combination of the two sets of lattice vectors that form the dichromatic pattern associated with the given GB of interest [4]:

$$\boldsymbol{R}^{DSC} = m\boldsymbol{a}^1 + n\boldsymbol{a}^2 + p\boldsymbol{a}^3 + u\boldsymbol{q}^1 + v\boldsymbol{q}^2 + w\boldsymbol{q}^3, \tag{26}$$

where m, n, p, u, v, and w integers, while $\boldsymbol{a}^j$ and $\boldsymbol{q}^k$ are the sets of lattice vectors associated with the two lattices that form the dichromatic pattern. Using the Eq. (26) a DSC lattice can be generated and its primitive lattice vectors then determined.

CALCULATION OF BURGERS VECTOR OF GRAIN BOUNDARY PHASE JUNCTION

While any circuit can be drawn to find the Burgers vector, from a practical point of view, in general, the simpler the circuit, the easier it is to calculate. Such a circuit is shown schematically in Fig. 5a, depicting a grain boundary phase junction, but with a simplified Burgers circuit. The Burgers circuit in Fig. 5a consists of four vectors: $\boldsymbol{v}^T$ and $\boldsymbol{v}^B$, which do not cross the grain boundary; $\boldsymbol{v}^\beta$ and $\boldsymbol{v}^\alpha$, which cross the grain boundary through the β and α phase respectively.

The Burgers circuit is the closure failure of the circuit after the current system has undergone cuts in the material. One cut, or many can be used. In the case of the phase junction shown in Fig. 5a we will proceed by making a cut in the material such that the result of this cut is that $\boldsymbol{v}^\beta \to \boldsymbol{V}^\beta$, $\boldsymbol{v}^T \to \boldsymbol{V}^T$, $\boldsymbol{v}^\alpha \to \boldsymbol{V}^\alpha$ and $\boldsymbol{v}^B \to \boldsymbol{V}^B$; where $\boldsymbol{V}^T$ and $\boldsymbol{V}^B$ are lattice vectors of equal length, while $\boldsymbol{V}^\beta$ and $\boldsymbol{V}^\alpha$ are the vectors crossing the grain boundary phases when mapped to a bicrystal with only an β or α phase present. Applying the transformation rule explained above gives

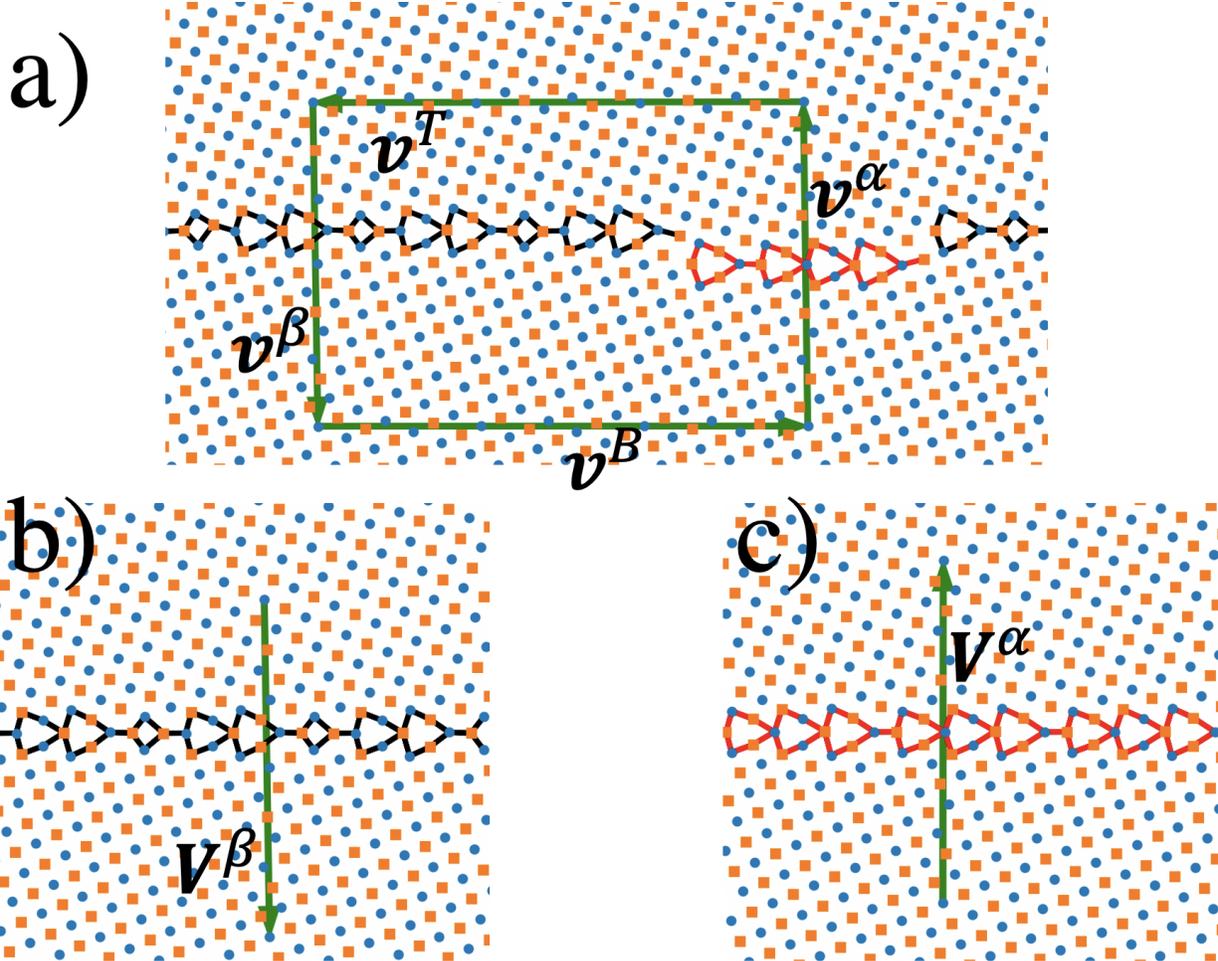$$\boldsymbol{b} = -\boldsymbol{V}^\alpha - \boldsymbol{V}^\beta. \tag{27}$$

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FIG. 5. Illustration of Burgers circuit used to calculate the Burgers vector of the grain boundary phase junction. Panel a depicts a closed circuit in the current system. Panel b shows the vector v^{β} in Panel a transformed into the reference system. Panel c shows the vector v^{α} in Panel a transformed into the reference system.

When applying Eq. (27) the Burgers vector is found to be $\boldsymbol{b} = 0.600\text{Å}\hat{\boldsymbol{e}}_1 + 0.423\text{Å}\hat{\boldsymbol{e}}_3$ from the specific system analyzed in the main text.

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* winter24@llnl.gov

† frolov2@llnl.gov

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