On the Twinnability of Face-Centered Cubic Metals in Deformed Microstructures

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ABSTRACT

The competition between deformation twinning and dislocation slip underpins the evolution of mesoscale plasticity in face-centered cubic materials. While competition between these mechanisms is known to be related to the critical features of the generalized stacking fault energy landscape, a physical theory that tracks competition over extended plasticity has yet to emerge. Here, we report a methodology to predict the evolution of this competition in deformed microstructures using intrinsic material parameters. Our approach implements kinetic Monte Carlo simulations and analytical modeling to produce a constitutive framework for deformation twin evolution in face-centered cubic metals that is free of empirical fitting or phenomenology. These efforts are leveraged to derive a set of physical relations for strain partitioning, which provide kinetically-weighted predictions for the contributions of each mechanism to plasticity. The culmination of this effort results in a new twinnability parameter that tracks the competition between deformation twinning and dislocation slip over extended plastic deformation. In contrast to previous twinnability parameters, this criterion considers deformation history when weighing mechanistic competition. This parameter therefore extends previous theories for the competition between these mechanisms to include deformation beyond incipient events. This analysis finds direct applications in work hardening and crystal plasticity models that have previously relied on

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phenomenological relations to predict the evolution of deformation twin microstructures.

Keywords: Deformation twinning; Twinnability; Crystal plasticity; Stacking fault energy; Kinetic Monte Carlo Simulations

1. INTRODUCTION

The mesoscale plasticity of face-centered cubic (FCC) metals is underpinned by the operation of competing deformation mechanisms. Amongst these, dislocation slip and deformation twinning are widely recognized to be two important mechanisms that actively compete during plastic deformation. The comparative dominance of one mechanism is determined by a complex interplay between intrinsic material properties and extrinsic factors. Competition in the former category can be conceptualized using the generalized stacking fault energy (GSFE) landscape, as described by Vítek.\cite{1} Various investigators have leveraged the GSFE landscape concept to produce parameter-based descriptors of mechanistic competition. For competition between deformation twinning and slip, Tadmor and co-workers provided the seminal descriptors. Their earliest work defines a twinning tendency criterion for the onset of deformation twinning at a crack-tip \cite{2}. Notably, this work demonstrated a nuanced relationship between the critical GSFEs (\textit{i.e.}, the unstable stacking fault and twinning energies) and deformation twinning, which challenged the general belief that twinning tendency is driven solely by the intrinsic stacking fault energy. A subsequent work broadened this approach by homogenizing the crack-tip model over a distribution of crack orientations in a polycrystal \cite{3}. Asaro and Suresh \cite{4} considered a specific slip system geometry, under the crack-tip parameter of Tadmor and Hai, to rationalize the competition between deformation twinning and slip at grain boundaries in nanostructured FCC materials. Jin et al. \cite{5} reparameterized the criterion of Asaro and Suresh to provide a single-parameter relation for twinning tendency under the original analytical framework of Tadmor and co-workers. In an
independent approach, Jo et al. [6] consolidated considerations of crystal orientation and GSFEs to develop a unified parameter that predicts tendencies for deformation twinning, slip, and stacking fault emission. These descriptors of competition between deformation twinning and slip are referred to here as ‘twinningability’ parameters following the nomenclature of Tadmor and Bernstein [3]. Each of these parameters are summarized in a recent review from De Cooman et al. [7].

While these twinnability parameters provide fundamental understanding of the intrinsic competition between deformation mechanisms, there are some notable limitations. Namely, these descriptors offer insight into incipient deformation tendencies (i.e., the first emission of an extended dislocation or formation of a twin embryo) but do not track competition as deformation evolves. This restriction on twinnability parameters inhibits their practical utility. For instance, the mixed operation of deformation twinning and dislocation slip is well-known to underpin the work hardening behavior of several high-performance metallic systems. Examples are found in a diverse set of technologically important systems including nanotwinned materials [8–10], high entropy alloys [11], and most notably in twinning-induced plasticity (TWIP) steels [12,13]. The engineering relevance of the deformation twinning mechanism has led to a rise in theoretical modeling efforts seeking to incorporate deformation twinning into work hardening laws. Early work from Rémy serves as the first effort in this area, where the deformation twin is considered as an obstacle that reduces the crystal mean free path [14]. Bouaziz and coworkers incorporated Rémy’s concept into a single-parameter dislocation density model using the Kocks-Mecking [15] framework to predict the work hardening behavior of TWIP steels [16–20]. A central component of Bouaziz’s model is an incremental strain partitioning rule that accounts for the relative contributions of dislocation slip and deformation twinning to overall crystal plasticity. The behavior of this strain partitioning rule is underpinned by an empirical law for the evolution of the
twin fraction, which is derived from the work of Olson and Cohen [21]. Subsequent efforts from several investigators have led to the incorporation of multiple dislocation density parameters [22–24] and kinematic hardening effects [18,25] into work hardening relations. In addition to internal parameter models, several crystal plasticity micromechanical models have also been proposed based on the seminal work of Kalidindi [26,27]. Notable examples are found in reports from Shiekhelsouk et al. [28], Barbier et al. [29], and Dancette et al. [30]. However, a persistent shortcoming in each of these approaches remains the lack of a physical expression for the evolution of the twin fraction. Consequently, predictions for deformation twin evolution have varied significantly. For instance, early empirical modeling efforts estimate a twin fraction as high as 0.69 in TWIP steels [16]. Later works have predicted a twin fraction in the range of ~0.10-0.20 [18,31], with 0.15 being the commonly accepted value [7]. While these later efforts better align with experimental observations, the broad applicability of current evolution models remain poor due to their reliance on phenomenology and empirical fitting.

The absence of a physical law for deformation twin evolution reflects the limitations noted in the previous discussion. Namely, descriptors of competition consider only incipient events and are therefore not predictive of changes in tendencies for deformation twinning or dislocation slip as deformation proceeds. Here, we present a methodology to reconcile these shortcomings. The relative competition between deformation twinning and dislocation slip is studied using kinetic Monte Carlo (kMC) simulations. Based on kMC simulations, a physical model is derived that leverages the critical energies of the GSFE landscape to predict mechanistic competition. The outcomes of this study are two-fold. The primary result provides a new parameter that predicts the competition between deformation twinning and dislocation slip over extended plastic deformation. From a fundamental perspective, this contribution expands the twinnability framework originally
developed by Tadmor and coworkers [2,3] by extending its scope beyond incipient events. Additionally, the analytical framework developed herein is leveraged to provide a first principles-based, physical model for the evolution of deformation twin fraction in FCC materials. We anticipate that this result will enhance existing work hardening and crystal plasticity models of deformed microstructures.

2. METHODOLOGY

2.1. Kinetic Monte Carlo approach

To address the question of mechanistic competition, we have implemented the relevant kinetic equations for dislocation slip and deformation twinning mechanisms using the algorithm outlined in Bortz et al. [32]. The kMC approach enables the analysis of a discretized crystal, where the nucleation and progression of defects is considered by traversing system states that are separated by kinetic barriers. These features are well-suited to the objectives of this work, which require tracking defects over extended deformation and monitoring the relative rate kinetics between deformation mechanisms. Following our previous work [33], the kMC simulation cell is considered as a FCC single crystal that is initially deformation free with the <112> and <111> crystallographic axes oriented along the global $x$ and $y$ direction, respectively. This orientation was selected to facilitate tracking of the twin fraction, $F$, from a $<110>$ zone axis. The simulation cell measures $M\vec{b}_{112}$ by $Nd_{111}$ where $\vec{b}_{112}$ is the magnitude of the $<112>$-type Shockley partial dislocation and $d_{111}$ is the interplanar distance between $\{111\}$ planes. The simulation cell possesses free surfaces along the $x$ axis and periodic boundaries along the $y$ axis. A schematic of the kMC simulation cell is provided in Figure 1a.

Two different kinetic processes are evaluated in kMC simulations: partial dislocation nucleation and partial dislocation glide. The operation of each of these processes is separately
considered for leading and trailing Shockley partial dislocations. Thus, mechanistic competition is determined by the sequential activation of the relevant processes required to trigger deformation twinning or dislocation slip. In order to provide an intrinsic comparison, extrinsic factors such as Schmid effects are removed, and we evaluate competition along a single twinning/slip system. In this work, we evaluate a boundary/surface-mediated mechanism for the formation of deformation twins through the nucleation and glide of leading \(<112\>-\)type Shockley partials. The incipient nucleation event of a leading partial forms an intrinsic stacking fault (ISF). Subsequent leading partial nucleation events on adjacent \{111\} slip planes lead to the formation of a two-layer extrinsic stacking fault (ESF) and a multi-layer twin fault (TF). Dislocation slip proceeds through the nucleation and glide of trailing \(<112\>-\)type Shockley partials at locations in the simulation cell where a fault structure already exists. This process causes layer-by-layer decrements to the thickness of ESF and TF defects (i.e., detwinning), or the restoration of the defect-free, slipped FCC lattice when an ISF is removed (see Figure 1a). All leading dislocations considered in this study were 90° edge-type Shockley partial dislocations. Two different 30° mixed Shockley partial dislocation variants were considered for trailing nucleation. The variants were determined from the two possible dissociation pairs that accompany the 90° leading partial to form a 60° \(<110\>-\)type extended dislocation, from which dislocation slip proceeds. To preserve an intrinsic study of a single twin/slip system, cross-slip mechanisms and detwinning and slip within the interior of fault structures are not considered.

The boundary-mediated partial dislocation emission mechanism implemented in this study can be seen as a logical extension of the crack-tip problem considered by Tadmor and coworkers [2,3]. However, to facilitate an intrinsic comparison of deformation mechanisms over extended plasticity we have replaced the crack-tip with a crystal surface. This boundary-mediated twin formation
mechanism is established in the experimental literature for a diverse set of systems including TWIP steels [13], nanostructured FCC materials [34–36], and hexagonal close-packed metals [37]. Furthermore, we have validated our implementation of the boundary-mediated nucleation mechanism against molecular dynamics simulations of deformation twin evolution in FCC nanowires [33]. The nucleation mechanism studied herein is distinct from other classical deformation twin formation theories such as the Cohen-Weertman [38] and Fujita-Mori [39] cross-slip mechanisms and the pole-based mechanism of Venables [40], but bears some similarities to the three-layer twin nucleus mechanism of Mahajan and Chin [41]. One notable distinction in our approach is that the nucleation of deformation twins is considered as a homogeneous phenomenon, where our system is agnostic of local microstructural heterogeneities (e.g., crack-tips, grain boundary energies) that may bias mechanistic competition. This treatment therefore has the intended effect of providing an intrinsic comparison of deformation mechanisms that arise explicitly from their various process barriers. Our approach is similar to that of Jo et al. [6], where a homogeneous treatment was used to study the competition between incipient mechanisms. Heterogeneities may only arise here due to fault structures that emerge from the deformation history. Yet, it should be noted that the kMC approach is sufficiently general such that microstructure heterogeneities can be specified, if desired.

The process barriers for partial dislocation nucleation are explicitly defined here using the critical energies of the GSFE landscape (see Figure 1b), following the method of Ogata et al. [42]. In this approach, the barrier that acts at the $j$th slip plane within the crystal is determined by the local fault environment and thus reflects the deformation history of the system (see Figure 1a). We have selected four common FCC materials (Ag, Au, Cu, and Al) for kMC simulations, for which the GSFE landscape is well-known. This selection was found to encompass the extremes in the
behaviors of mechanistic competition. Deformation twinning initiates with the incipient nucleation barrier \( (E_1^+) \) for a leading \(<112>\)-type Shockley partial dislocation. Thickening of deformation twins proceeds by overcoming additional process barriers \( (E_2^+, E_3^+, \ldots, E_n^+) \) that are defined as the difference between the relevant fault (i.e., \( \gamma_{isf}, \gamma_{esf}, \gamma_{tf} \)) and the peak energies (i.e., \( \gamma_{usf}^{1}, \gamma_{usf}^{2}, \gamma_{utf}^{3}, \gamma_{utf}^{\infty} \)) of the subsequent defect along the GSFE landscape. Similarly, the reverse parameters \( (E_1^-, E_2^-, E_3^-, \ldots, E_n^-) \) describe the process barriers for the nucleation of trailing \(<112>\)-type Shockley partial dislocations, which activate dislocation slip. The peak energies \( \gamma_{usf}^{1} \) and \( \gamma_{usf}^{2} \) refer to the unstable fault energies that must be overcome to form an ISF and an extrinsic stacking fault ESF, respectively. Similarly, the peak energies of \( \gamma_{utf}^{3} \) and \( \gamma_{utf}^{\infty} \) define the peak energies for an embryotic and thickened deformation twin, respectively. In each case, the superscript refers to the number of leading dislocations required to form the relevant fault structure. Table 1 provides the values for the critical energies of the GSFE landscape (i.e., \( \gamma_{usf}^{1}, \gamma_{usf}^{2}, \gamma_{utf}^{3}, \gamma_{utf}^{\infty} \)) used in kMC simulations. These values are obtained from density functional theory calculations using the climbing-image nudged elastic band method, as reported in Jin et al. [5]. The zero Kelvin energies are used in this study, as is normal practice, given the lack of reliable measurement of the GSFE landscape at finite temperature. In FCC metals, the critical energies of the GSFE landscape are known to stabilize after the formation of an ESF [42], which can be considered as a twin embryo with two adjacent twin boundaries. Therefore, the process barriers for twinning \( (E_3^+) \) and detwinning \( (E_3^-) \) of the twin embryo are determined using the approximation \( \gamma_{utf}^{3} \approx \gamma_{usf}^{2} \). The energy of the three-layer twin embryo is taken as \( \approx 2\gamma_{tf} \), where \( \gamma_{tf} \) is the energy of an isolated coherent twin boundary. The process barrier for twinning and detwinning at thicknesses of beyond three \(<111>\) planes is defined by \( E_{\omega}^{+} \) and \( E_{\omega}^{-} \), respectively. Each of these approximations are
common within the community, as discussed in Jin et al. [5] and De Cooman et al. [7].

Following the kMC method, the rates ($R_{i,j}$) of nucleation and glide events are calculated using the Arrhenius relation:

$$R_{i,j} = R_o \exp \left\{ -\frac{(\hat{\sigma}_{i,j} - \sigma_{i,j})V}{k_b T} \right\}$$

(1)

where $R_o$ is the Debye frequency, $V$ is the activation volume (taken as $10 \bar{b}^3$, as per Ramachandramoorthy et al. [43]), $k_b$ is the Boltzmann constant, and $T$ is the temperature (set at 300 K). $\hat{\sigma}_{i,j}$ and $\sigma_{i,j}$ are the process barrier and elastic stresses, respectively, that operate at the $i^{th}$ activation site in the $j^{th}$ slip plane of the kMC simulation cell. The values for $\sigma_{i,j}$ are updated at each step of the kMC simulation depending on the local deformation history. For instance, in a pristine simulation cell $\hat{\sigma}_{i,j}$ reduces to $\hat{\sigma}_{0,j}$, which defines the stress to nucleate a leading $<112>$-type Shockley partial dislocation. After nucleation of a leading partial in the $j^{th}$ slip plane, $\hat{\sigma}_{0,j}$ then becomes the stress to nucleate a conjugate $<112>$-type trailing partial (for dislocation slip) and $\hat{\sigma}_{i,j}$ is the stress required for glide of the leading partial at the $i^{th}$ activation site (i.e., the Peierls-Nabarro stress, $\sigma_{PN}$, see Figure 1a). These nucleation and glide stresses are then updated as the kMC simulation proceeds, to reflect the local fault environment. When glide is operative, the process barrier stress may be calculated from the solution to the Peierls-Nabarro problem for a partial dislocation [44]. Following the analysis of Ogata et al. [42], the undulations of the GSFE landscape can be considered as a Peierls potential and may used to directly determine process barrier. These considerations lead to a conditional definition for the process barrier stress $\sigma_{i,j}$:
\[
\hat{\sigma}_{l,j} = \begin{cases} 
\frac{\pi E_{l,j}}{b_{112}}, & \text{nucleation} \\
\frac{2\pi \zeta_{p(l,j)}}{\rho} \exp \left(-\frac{2\pi \zeta_{p(l,j)}}{\rho}\right), & \text{glide}
\end{cases}
\]

where \(E_{l,j}\) is the process barrier for leading or trailing nucleation in the relevant fault environment and \(\zeta_{p(l,j)} = \frac{K_{p}b_{112}^{2}}{4\pi^{2}E_{l,j}}\) is the half-width of the dislocation core. \(\rho\) is a geometric parameter that takes the value of \(\sqrt{3} \frac{b}{b_{112}}\) for a screw dislocation or \(\frac{3}{2} \frac{b}{b_{112}}\) for an edge dislocation, and \(b_{p}\) is the magnitude of the edge or screw component of the \(<112>\) Shockley partial dislocation. \(K_{p}\) is an elastic constant that is defined by the shear modulus \((G)\) and the Poisson’s ratio \((\nu)\) as \(K_{p} = G\) or \(K_{p} = \frac{G}{1-\nu}\) for screw and edge dislocations, respectively. Glide barriers for \(30^\circ\) trailing partial dislocations are computed from the component-wise solution to the Peierls-Nabarro model for its screw and edge components [42,44]. The relevant material parameters used in all kMC calculations are provided in Table 1. The effective process barrier stress (i.e., \(\hat{\sigma}_{l,j} - \sigma_{l,j}\)) is determined by considering the additive contributions of elastic stress fields from partial dislocations stored in the kMC simulation cell. Individual stress fields are calculated using the Volterra solution to the dislocation elasticity problem for each leading and trailing partial dislocation [45]. The relevant stress tensors are transformed to align with the Burger’s vectors of the respective defect (i.e., \(90^\circ\) or \(\pm 30^\circ\) partial dislocations). Nucleation of conjugate \(\pm 30^\circ\) trailing partial dislocations therefore offers two effective process barrier stresses for consideration in the same kinetic move. Boundary effects are accounted for using the image dislocation method, which enforce a vanishing condition along free surfaces (i.e., the \(<112>\) surfaces of the kMC simulation). Further details on the dislocation elasticity calculations performed in this study are provided in the Supplementary Material. In addition to stresses arising from internal defects, the application of external far-field
loadings can reduce the effective process barriers. The effects of far-field loadings are not specifically considered here as they exert a uniform influence on rate kinetics. However, it should be noted that our formulation is sufficiently general to include their effects along with the associated Schmid factors.

Implementation of Eqs. (1) and (2) within the kMC method enables a kinetically-weighted observation of deformation phenomena where the likelihood of twinning and slip is determined by the deformation history. At each simulation step, the twin fraction \( F \) and number of twins \( N_T \) are measured from a lineal section of the simulation cell. The calculation of the deformation twin fraction and twin number also includes contributions from single and two-layer defects such as ISFs and ESFs, which is consistent with the treatment of the deformation twinning mechanism sequence in previous works [2,3,42]. For this reason, we use the terms defect, fault, and twin interchangeably throughout the results and discussion. The simulation cell is initialized in a pristine condition and simulations are terminated once the plastic strain \( \gamma_p \) reaches 0.2. Plastic strain is calculated here as a shear strain relative to the \(<112>\) and \(<111>\) crystal axes (i.e., \( \gamma_{xy} \) relative to the global \( x \) and \( y \) axes). Therefore, the annihilation of a leading and trailing partial dislocations at the right boundary contributes increments of \( \frac{1}{\sqrt{2}} |dF| \) and \( \frac{1}{2\sqrt{2}} |dF| \) to the cumulative plastic strain, respectively, where \( |dF| = \frac{1}{N} \).

### 2.2. Analytical model

An analytical model has been developed to track the competition between deformation twinning and dislocation slip over extended plasticity. The intended outcome of this effort is a physical description for the partitioning of the twin fraction with plastic strain. This model consists of a system of coupled equations that can be solved using standard numerical techniques. This
The evolution of twin fraction can be quantified as the summation of the twin fraction increment \( \frac{dF^+}{d\gamma_p} \) and decrement \( \frac{dF^-}{d\gamma_p} \) per increment of plastic strain:

\[
\frac{dF}{d\gamma_p} = \frac{dF^+}{dN_L} \frac{dN_L}{d\gamma_p} + \frac{dF^-}{dN_L} \frac{dN_L}{d\gamma_p}
\]

where \( \frac{dN_L}{d\gamma_p} \) is the incremental change in the number of nucleated dislocations per increment of plastic strain. The terms \( \frac{dF^+}{dN_L} \) and \( \frac{dF^-}{dN_L} \) are related to the probability that a nucleation event (i.e., an increment to the number of nucleated dislocations, \( dN_L \)) results in an increase or decrease to the twin fraction, respectively. These terms may be determined directly from the probabilities for leading \( (P^+) \) and trailing nucleation \( (P^-) \):

\[
\frac{dF^+}{dN_L} = P^+ |dF| \quad (4a)
\]

\[
\frac{dF^-}{dN_L} = -P^- |dF| \quad (4b)
\]

By inspection, the nucleation probabilities define the likelihood of an incremental or decremental change to the twin fraction (i.e., \( |dF| = \frac{1}{N} \)) and by definition \( P^+ \) and \( P^- \) fall in the range of 0 to 1.

The twin fraction therefore evolves at partial increments of \( -\frac{1}{N} \leq dF \leq \frac{1}{N^*} \) which reflects the weightings of leading and trailing nucleation probabilities. As shown in our previous work [33], the probabilities for these events may be derived from proportion of leading \( (R^+) \) and trailing \( (R^-) \) to the total rates \( (R) \) summed over all activation sites in the kMC model:

\[
P^+ = \frac{R^+}{R} \frac{[N - FN - 2N_T E_1^+ + 2N_T E_2^+ + 2N_1 E_1^+ + 4N_{\omega} E_2^+]}{[N - FN - 2N_T E_1^+ + 2N_T E_2^+ + 2N_1 E_1^+ + 4N_{\omega} E_2^+]}
\]

(5a)
\[
P^{-} = \frac{R^{-}}{R} = \frac{2N_{1}\bar{E}_{1}^{-} + 4N_{\infty}\bar{E}_{2}^{-}}{[N - FN - 2N_{T}]E_{1}^{+} + 2N_{T}E_{2}^{+} + 2N_{1}E_{1}^{-} + 4N_{\infty}E_{2}^{-}} \tag{5b}
\]

where \(N_{1}\) and \(N_{\infty}\) are the number of single- (i.e., ISFs) and multi-layer faults (i.e., ESFs and TFs), respectively. \(\bar{E}_{k}^{l}\) is the relevant leading or trailing barrier coefficient such that \(\bar{E}_{k}^{l} = \exp \left\{ \frac{-\nu_{l}}{k_{B}Tb_{112}}E_{k}^{l} \right\}\). Here, we have neglected elastic stresses and implemented the approximation \(E_{2}^{+} \approx E_{3}^{+} \approx E_{\infty}^{+}\) and \(E_{2}^{-} \approx E_{3}^{-} \approx E_{\infty}^{-}\), which follows from our previous work [33]. The coefficients preceding the trailing rates reflect the opportunity for the nucleation of two trailing partial dislocation variants. The evolution equations for \(N_{T}, N_{1}\), and \(N_{\infty}\) are discussed below. Lastly, an evolution law is required to account for the differing contributions of leading and trailing partials to the plastic strain. The differential partitioning of the overall plastic strain is expressed as:

\[
\frac{d\gamma_{P}}{dN_{\perp}} = \frac{1}{\sqrt{2}} \left( P_{L} + \frac{P_{T}}{2} \right) |dF| \tag{6}
\]

The evolution of deformation twinning morphologies, \(N_{1}\) and \(N_{\infty}\), is assessed as part of a model to predict the twin number density (i.e., \(n_{T} = \frac{N_{T}}{N}\)). We consider two outcomes that can alter the number of twins – namely, the nucleation of a leading and trailing partial dislocation. As in the twin fraction model, the evolution in the number of twins with plastic strain is described by a similar additive relation:

\[
\frac{dN_{T}}{d\gamma_{P}} = \frac{dN_{T}^{+}}{dN_{\perp}} \frac{dN_{1}}{d\gamma_{P}} - \frac{dN_{T}^{-}}{dN_{\perp}} \frac{dN_{\infty}}{d\gamma_{P}} \tag{7}
\]

where \(\frac{dN_{T}^{+}}{dN_{\perp}}\) and \(\frac{dN_{T}^{-}}{dN_{\perp}}\) are related to the probabilities of an increase or decrease to the number of twins, respectively. To model the probability of an increase to the number of twins, we consider the comparative kinetics of these outcomes as deformation proceeds. Specifically, an increase to
only occurs when a leading partial dislocation is nucleated in a defect-free area of a crystal and a decrease to \( N_T \) is accompanied by the nucleation of a trailing partial dislocation at an ISF. The relevant quantities are defined as follows:

\[
\frac{dN_T^+}{dN_1} = \frac{[N - FN - 2N_T]E_1^+}{[N - FN - 2N_T]E_1^+ + 2N_TE_2^+ + 2N_1E_1^- + 4N_\infty E_2^-} \quad (8a)
\]

\[
\frac{dN_T^-}{dN_1} = \frac{2N_1E_1^-}{[N - FN - 2N_T]E_1^+ + 2N_TE_2^+ + 2N_1E_1^- + 4N_\infty E_2^-} \quad (8b)
\]

In order to solve Eqs. (8a) and (8b), a rule for the partitioning of twin morphologies is required. The evolution of these quantities is described by the following relation:

\[
\frac{dN_\infty}{dN_1} = \frac{2N_1E_2^+ - 4N_\infty E_2^-}{[N - FN - 2N_T]E_1^+ + 2N_TE_2^+ + 2N_1E_1^- + 4N_\infty E_2^-} \quad (9a)
\]

\[
N_1 + N_\infty = N_T \quad (9b)
\]

which accounts for the growth in the number of multi-layer twins due to thickening of ISFs and its decrease due to detwinning.

The ratio of the probabilities for leading and trailing partial dislocation nucleation is also of interest, given the influence that these parameters have on mechanistic competition. We define here the competition parameter (\( \eta \)) as the ratio of leading and trailing probabilities as:

\[
\eta = \frac{P^+}{P^-} = \frac{[N - FN - 2N_T]E_1^+ + 2N_TE_2^+}{2N_1E_1^- + 4N_\infty E_2^-} \quad (10)
\]

Examination of Eq. (10) offers interesting insights. For instance, the relevant process barriers \( i.e., E_1^+, E_2^+, E_1^- \) and \( E_2^- \) contain the GSFE parameters \( i.e., \gamma_{usf}^1, \gamma_{usf}^2, \gamma_{isf} \) that are found in the incipient twinnability parameter of Tadmor and co-workers [2,3]. However, here we have also
implemented additional variables \((i.e., F, N_1, N_\infty, \text{ and } N_T)\) that account for the evolution of the microstructure during deformation. Collectively, Eqs. (3)-(10) provide a first principles-based physical framework to predict the evolution of mechanistic competition over extended plasticity in FCC materials, without the need for the empirical fitting or phenomenology.

### 3. RESULTS AND DISCUSSION

The kMC model described in Section 2.1 has been implemented to study the mechanistic competition in a variety of crystal sizes for Ag, Au, Cu, and Al. The results for kMC systems measuring \(300\vec{b}_{112} \times 300d_{111}\) for Ag, Au, and Cu form the basis of the analysis presented in the main text. kMC simulations of Al do not exhibit deformation twinning but are provided in the Supplementary Material for model validation purposes. Each kMC simulation condition has been replicated 100 times for statistical sampling and was observed to converge well below the replication limit. All error bars are reported as \(\pm 1\) standard deviation. All contour plots are normalized from a binning strategy performed on the kMC simulation results. The raw kMC data is binned along the \(x\) and \(y\) axes of the plot and bin counts are presented as normalizations of the maximum measurements along the plot ordinate. The coupled analytical equations are sequentially solved using the 4\(^{th}\) order Runge-Kutta numerical method. Additional results examining size effects, deformation twinning in Al, and a sensitivity analysis of kMC replications are provided as Supplementary Material.

#### 3.1. Evolution of deformed microstructures

Representative snapshots of the kMC simulation cell at several stages of plastic deformation are shown in Figure 2 for Ag, Au, and Cu. The shaded stroke represents regions where a fault is currently present. As anticipated, several fault structures \((i.e., \text{ISFs}, \text{ESFs}, \text{and TFs})\) are progressively nucleated and annihilated during plastic deformation. Ag exhibited the highest
storage of faults, whereas faults nucleated in Cu were found to be rapidly annihilated by the emission of a trailing partial dislocation. In each material, the storage of fault structures was observed to approach saturation by $\gamma_p \approx 0.15$. Videos of the evolution of deformed microstructures with increasing plastic strain are made available as Supplementary Material. The deformation processes and morphologies presented in Figure 2 are qualitatively substantiated by tensile experiments of single crystal nanowires. Although experimental studies inherently probe loading orientation factors (i.e., Schmid effects), which are intentionally neglected herein, single-crystal nanowires represent a reasonable system for comparison to kMC simulations as they possess analogous boundary conditions (i.e., free surfaces). Ramachandramoorthy et al. [43] observed the nucleation and storage of thin twin lamellae ($< 5d_{11\bar{1}}$) in nanotensile experiments single crystal Ag nanowires. Lee et al. [36] observed partial dislocation-mediated twinning and detwining mechanisms in Au nanowires subjected to cyclic tensile/compressive loadings. These experimental reports correlate well with the deformation structures observed in kMC simulations.

Figure 3 presents the evolution of the twin number density for each material in the study. The raw data from all replications of the kMC simulations is provided as normalized contours, as described above, and the averaged data is plotted using the relevant markers. Analytical predictions from the model defined in Section 2.2 are plotted in dashed stroke. For each material, the model predictions of twin number density evolution fall well within the error bars of kMC simulations. Indeed, the agreement between the model and the average kMC data for Ag is excellent. Deviations from the average kMC data for Au may be explained through consideration of the kMC raw data (contours), which highlight the effect of data scatter. It should be noted that the scatter in data is asymmetric, as the twin number density cannot fall into negative values. The most common occurrence (dark red regions) in these kMC simulations does not necessarily match with the kMC
average for Au. Nonetheless, the most common occurrence is captured here by the analytical model. Similarly, in the case of Cu, the analytical model predicts a twin number density that lies between the two most common events – namely, a simulation cell with a single ISF or the defect-free condition. As with Au, the average of kMC data is shifted upwards by isolated incidences of large twin number densities. Additional results showing the kMC data and model predictions for fault morphologies (i.e., $N_1$ and $N_\infty$) are provided in the Supplementary Material.

The evolution of the twin fraction with increasing plastic strain for Ag, Au, and Cu is plotted in Figure 4. As with the twin number density plots, the average kMC data, contoured raw data, and model predictions are presented. In each material, a monotonic increase in the twin fraction is predicted, with Ag exhibiting the highest defect storage. Again, the analytical model is in very good agreement and captures the critical features of the kMC simulation data. Deviations between average kMC data and model predictions are again attributed to asymmetric scatter in the kMC simulation data. Ag exhibits the best match to model predictions as scattering in the twin fraction data is most symmetric. In each material, the rate of increase in the twin fraction is highest at incipient stages of plasticity and approaches a linear relation at higher plastic strains. Cu and Au exhibit only very meager increases in the twin fraction after 0.01-0.02 plastic strain, whereas Ag tends to continue to store twin defects at higher strains, albeit at a reduced rate. This behavior is in line with the experimental literature, which reports a steep increase in the twin fraction during incipient plastic events [7].

The ability of the analytical model to capture the evolution of the twin fraction over extended plasticity is perhaps the most notable outcome of these results. Indeed, using only process barriers derived from the GSFE landscape, we have developed a first principles-based methodology that can predict the partitioning of contributions (i.e., deformation twinning vs slip) to plastic strain for
several FCC materials. This physical description of the strain partitioning phenomenon is free from empirical fitting and is anticipated to improve the phenomenological relations currently implemented in work hardening and crystal plasticity models. Examples, where a direct application of this approach would be beneficial, are found in the dislocation storage framework of Bouaziz and coworkers [16–20] and deformation twinning crystal plasticity models, [28–30] among others.

While we anticipate that the outcomes of these efforts will be of interest to the community, it is also important to highlight some of the caveats in the application of this method. Namely, we expect that this physical model is most applicable in cases where microstructural heterogeneities (e.g., crack-tips) are not readily available to cause localization of deformation. Furthermore, we recognize that the assumptions undertaken in model development merit a discussion of verification. Therefore, in addition to previous validation efforts [33], we have independently verified the kMC approach and physical model developed herein. For this purpose, the kMC method has been leveraged to calculate the stacking fault width between dissociated partial dislocations in Al. Here, kMC simulations result in an average stacking fault width of 1.06 nm, which is in excellent agreement with the analytical solution of 0.92 nm from dislocation theory [45]. Further details of this validation effort are provided as Supplementary Material.

### 3.2. Twinnability under extended deformation

The results of the kMC simulations and analytical modeling may also be used to investigate the twinnability of FCC materials over extended plastic deformation. Figure 5 presents the evolution of the competition parameter, $\eta$, with twin fraction. The analytical model (Eq. (10)) is plotted in dashed stroke for each material. Additionally, two bounding cases for the analytical model are considered (solid stroke) that result in the upper ($\eta_u$) and lower ($\eta_l$) estimates for $\eta$. 

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These parameters are included to contextualize the scatter in the contour data. Further details for the calculation of $\eta_u$ and $\eta_l$ are provided as Supplementary Material. In a small minority of cases for Cu and Au, the kMC data falls outside of the established analytical bounds. This is due to the effect of shear stresses from dislocations that operate on the nucleation barriers.

As shown in Figure 5, each of the materials exhibit a reduction in the competition parameter with increasing twin fraction. This finding is intuitive, as additional activation sites become available for trailing dislocation nucleation when more fault structures are present. The competition parameter is observed to be the largest for Ag across all twin fractions, whereas it quickly decreases towards unity for Cu and Au. The most common occurrences in the kMC data are well-captured by the bounding behaviors of the analytical model for each material under study. Deviations of model predictions from the average kMC values are due to asymmetries in the data scatter. Perhaps the most notable feature of the competition parameter data is that it enables the definition of twinnability that accounts for extended deformation in its formulation. For this purpose, we define the twinnability ($T_\eta$) as:

$$T_\eta = \ln(\eta) = \ln \left( \frac{[N - FN - 2N_T]E_1^+ + 2N_T E_2^+}{2N_1 E_1^- + 4N_\infty E_2^-} \right)$$

(11)

Here, deformation twinning is favored when $T_\eta > 0$ and slip is favored when $T_\eta < 0$. This twinnability parameter contains two distinct components that represent the material and microstructure parameters. Namely, within this parameter, the familiar intrinsic GSFE parameters (i.e., $\gamma_{usf}^{1}, \gamma_{usf}^{2}, \gamma_{isf}$) are embedded in the process barriers and the effects of deformation history are tracked in the microstructure evolution terms $F, N_1, N_\infty$ and $N_T$. The twinnability data for Ag, Au, and Cu is plotted in Figure 6a. Twinnability predictions from this parameter have also been compared against the parameters of Jo et al. [6], Jin et al. [5], Asaro and Suresh [4], and Tadmor
and Bernstein [3] in Figure 6b-f. The material parameters defined in Table 1 are used for all twinnability calculations. Incipient values of $T_\eta$ are plotted with markers, and the demarcation between twinning-dominated and slip-dominated behavior is denoted in a dashed stroke. Incipient data for Al has also been included to show alignment with other twinnability parameters in the slip-dominated regime. The incipient values of $T_\eta$ are calculated after the nucleation of an initial ISF (i.e., $F = \frac{1}{N}, N_1 = N_T = 1$), which aligns with the microstructures considered in the referenced parameters. Comparison with the literature parameters yields several interesting results. For instance, the sequencing of incipient values of $T_\eta$ (i.e., $T_\eta_{Ag} > T_\eta_{Cu} > T_\eta_{Au}$) is in agreement with the other literature parameters. Furthermore, our parameter predicts an important crossover in the twinabilities of Au and Cu after the incipient deformation stage. Wire drawing experiments from English and Chin have reported preferential twinning in Au relative to Cu [46]. This behavior is not captured by existing twinnability parameters but is exclusively revealed by $T_\eta$. Indeed, this discrepancy in twinnability predictions and experimental data is noted in the seminal work from Tadmor and Bernstein [3]. We also note that $T_\eta$ returns the same conditional inequalities as other twinnability parameters when the microstructural evolution parameters are omitted and process barrier definitions are aligned. For instance Jo et al. [6], defined twinnability process barriers using the relation $\frac{E}{\cos \theta}$, where $\theta$ is the angle between the dislocation Burger’s vector and the $\langle 112 \rangle$ twinning partial. For $\theta = 60^\circ$ (i.e., for a $30^\circ$ trailing partial dislocation) considered at comparable incipient conditions, $F = \frac{1}{N}, N_1 = N_T = 1, N - FN = 2N_T = 0$, and using the transformation $\gamma^2_{usf} \approx \gamma^1_{usf} + \frac{1}{2} \gamma_{isf}$ [5], the criterion for deformation twinning reduces to $\frac{\gamma_{isf}}{\gamma_{usf} - \gamma_{isf}} < 2$, which is the same inequality presented by Jo et al [6]. Through the development of this parameter, we have
demonstrated a method to predict the twinnability of FCC metals by separately weighing the contributions of process barriers and deformation history to competition between deformation mechanisms. In a broad sense, we have expanded the application of the twinnability concept to describe the evolution of deformation twinning and dislocation slip in deformed microstructures.

4. CONCLUSIONS

The competition between deformation twinning and dislocation slip has been studied for four common FCC metals (Ag, Au, Cu, and Al) using kMC simulations. In contrast to previous efforts, which examine only incipient events, the evolution of mechanistic competition has been considered over extended plastic deformation. Kinetics in kMC simulations are informed directly by the critical features of the GSFE landscape and therefore provide an intrinsic comparison of mechanism competition. kMC simulations were implemented to track the evolution of the twin number density and the twin fraction. Results from these efforts show that Ag exhibited the highest storage of deformation twins and the highest twin fraction over the entire deformation range studied. Based on kMC results, an analytical framework has been developed to provide a physical model for the evolution of deformation twin microstructures in FCC metals. An interesting finding from analytical modeling is the observation of a crossover in the twinnabilities of Au and Cu after initial deformation events. The comparative ease of deformation twinning in Au has been previously reported in experimental studies, yet remains unexplained by the available parameters of deformation twinning theory. The outcomes of this study culminate in a new parameter that considers the contributions of process barriers and deformation history in the determination of twinnability. This new parameter therefore extends application of the twinnability concept to include deformed microstructures beyond the incipient stages of plasticity. Furthermore, the analytical framework derived herein forms the basis of a physical model for strain partitioning in
FCC metals. This first principles-based formulation is free from empirical fitting constants and may be implemented to improve current work hardening and crystal plasticity models, which have previously relied on phenomenology.

ACKNOWLEDGEMENTS

This work was supported by funding from the University of Illinois at Chicago. The authors would like to thank G. Hibbard for useful comments and suggestions on the manuscript.

AUTHOR CONTRIBUTIONS

M.D. conceived the project, co-wrote the manuscript, developed the kMC code, performed some of the kMC simulations, and derived the analytical model. R. J. co-wrote the manuscript and performed some of the kMC simulations.

ADDITIONAL INFORMATION

Supplementary information is available in the online version of the paper or by email request from the corresponding author (mattdaly@uic.edu).

COMPETING INTERESTS

The authors declare no competing interests.

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Figure 1: (a) The kMC simulation cell with the relevant crystal directions and geometric parameters noted. The signature fault structures of deformation twinning (i.e., ISF, ESF, and TF) and dislocation slip (i.e., a dissociated partial) are shown schematically. The nucleation barriers for deformation twinning and dislocation slip are shown in red and blue stroke, respectively. The determination of nucleation barriers is defined by the deformation history of the simulation cell. (b) The generalized stacking fault energy landscape for a typical FCC material. The relation between nucleation barriers and the local fault environment is illustrated. The values on the abscissa indicate the number of leading partial dislocations required to create each fault structure.
Figure 2: Snapshots from kMC simulations at plastic strains of 0.05, 0.1, and 0.15. The shaded regions indicate the presence of a fault. For Ag, the simulation cell is segmented by several fault structures. By contrast, deformation in Cu is slip-dominated and any planar faults are readily annihilated by the nucleation of trailing partial dislocations.
Figure 3: The evolution of twin number density as predicted by kMC simulations is overlaid with the analytical model (dashed line). The data is plotted for Ag (a), Au (b), and Cu (c). Error bars represent ±1 standard deviation over 100 replications of the kMC simulation. The raw kMC simulation data is shown in the contour plots. The contour plots are color-coded using a normalization scheme implemented along the ordinate axis. See the main text for further details.
Figure 4: The evolution of twin fraction as predicted by kMC simulations is overlaid with the analytical model (dashed lines). The data is plotted for Ag (a), Au (b), and Cu (c). Error bars represent ±1 standard deviation over 100 replications of the kMC simulation. The contour plots are color-coded using a normalization scheme implemented along the ordinate axis. See the main text for further details.
Figure 5: kMC predictions for the competition parameter are overlaid with the analytical model (dashed line). The bounding cases for the analytical model are shown in solid stroke. The data is plotted for Ag (a), Au (b), and Cu (c). The contour plots show the raw kMC data and are normalized relative to the maximum bin values at increasing twin fraction intervals. See the main text for details.
Figure 6: (a) The evolution of the twinnability parameter over extended deformation twinning is plotted for each material studied herein. (b) The twinnability parameter ($T_n$) is compared against the parameters of Jo et al. [6] (c), Jin et al. [5] (d), Asaro and Suresh [4] (e), and Tadmor and Bernstein [3] (f). The dashed line demarcates twinning- and slip-dominated regimes. Incipient data is plotted as a marker for each material and the data for Al (slip-dominated) is provided for comparison. In each case, the sequence of twinnability is in agreement.
### Table 1: Material parameters used in kMC simulations. Fault energies are provided in units of (mJ/m²).

| Material | $\bar{b}_{111}$ (nm) | $d_{111}$ (nm) | $G$ (GPa)$_a$ | $\nu$ | $R_o$ $(10^{13}$/s) | $\gamma_{usf}$ | $\gamma_{usf}^2$ | $\gamma_{isf}$ | $\gamma_{isf}^{\infty}$ | $\gamma_{esf}$ | $\gamma_{ef}$ |
|----------|----------------------|----------------|----------------|-----|-----------------------|----------------|----------------|----------------|----------------|----------------|-------------|
| Ag       | 0.167                | 0.236          | 25.5           | 0.39| 3.94                  | 91             | 100            | 93             | 16             | 12             | 8           |
| Au       | 0.167                | 0.235          | 24.1           | 0.43| 4.92                  | 68             | 79             | 72             | 25             | 27             | 12          |
| Cu       | 0.148                | 0.209          | 40.0           | 0.37| 7.98                  | 158            | 179            | 161            | 36             | 40             | 18          |
| Al       | 0.165                | 0.234          | 26.2           | 0.35| 9.66                  | 140            | 196            | 135            | 112            | 112            | 50          |

$_a$Calculated from compliance constants in Huntington [47] using a Reuss homogenizing assumption

$_b$Retrieved from Jin et al. [5]