Anisotropic failure behavior of ordered intermetallic TiAl alloys under pure mode-I loading

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Received 25 March 2020, revised 19 June 2020
Accepted for publication 17 July 2020
Published 14 August 2020

Abstract

Whether a metallic material fractures by brittle cleavage or by ductile rupture is primarily governed by the competition between cleavage and dislocation emission at the crack tip. The linear elastic fracture mechanics (LEFM) based criterion of Griffith, respectively the one for dislocation emission of Rice, are sufficiently reliable for determining the possible crack tip propagation mechanisms in isotropic crystalline metals. However, the applicability of these criteria is questionable when non-cubic, anisotropic solids are considered, as e.g. ordered intermetallic TiAl phases, where slip systems are limited and elastic anisotropy is pronounced. We study brittle versus ductile failure mechanisms in face-centered tetragonal TiAl and hexagonal Ti$_3$Al using large-scale atomistic simulations and compare our findings to the predictions of LEFM-based criteria augmented by elastic anisotropy. We observe that the augmented Griffith and Rice criteria are reliable for determining the direction dependent crack tip mechanisms, if all the available dislocation slip systems are taken into account. Yet, atomistic simulations are necessary to understand crack blunting due to mixed mechanisms, or shear instabilities other than dislocation emission. The results of our systematic study can be used as basis for modifications of the Griffith/Rice criteria in order to incorporate such effects.

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Keywords: intermetallics, titanium aluminides, molecular statics simulations, fracture mechanisms, anisotropic elasticity

(Some figures may appear in colour only in the online journal)

1. Introduction

Excellent combination of high specific strength, low density, and good structural stability makes titanium aluminides (TiAl alloys) promising candidates for aerospace structural materials even at high temperature [1]. However, TiAl alloys often exhibit in-service brittle failure behavior due to their low fracture toughness, and low fatigue strength at low temperatures [2–4]. This inherent brittleness significantly limits the applicability and industrial manufacturing of TiAl components. TiAl intermetallic alloys have significant bonding directionality that gives rise to highly anisotropic cleavage energy for crack propagation in different crystallographic planes of a TiAl microstructure [1, 9].

In general it is accepted that lamellar TiAl alloys, consisting of the tetragonal $\gamma$-TiAl (structure L10) and hexagonal $\alpha_2$-Ti$_3$Al (structure D019) phase, provide the best combination of strength and deformability. However, propagation of cleavage cracks leading to brittle fracture in lamellar TiAl alloys is still observed [5–7]. Particularly, $\gamma$-TiAl is found to be more susceptible to brittle fracture while $\alpha_2$-Ti$_3$Al exhibits a somewhat higher resistance to such crack growth. Sometimes cracks are even observed to be arrested at $\alpha_2$-Ti$_3$Al. But also deflection of cracks from $\gamma/\gamma$ interfaces for certain crystallographic orientations are shown in transmission electron microscopy (TEM) studies [5–7]. These observations demonstrate the pronounced anisotropy and low fracture toughness of both phases, $\gamma$, and $\alpha_2$. Indeed both phases possess a limited number of independent slip systems. Thus the competition between dislocation emission and cleavage at the crack tip is complex and strongly dependent on the crystallographic orientation of the crack. For an optimisation of the microstructure, the crack propagation mechanisms in the individual phases has to be understood first. Ideally, a relationship to the fundamental material parameters should be determined, to provide guidelines for alloying and processing strategies.

To this end, Yoo et al [8], calculated the Griffith energy ($G_c$) of different crystallographic planes of $\gamma$-TiAl with an ab initio density functional theory (DFT) method. They found significant anisotropy in the critical energy release rate. Panova et al [9] observed in molecular dynamics simulations, that also the mechanism of crack propagation in $\gamma$-TiAl is sensitive to the orientation of the crack with respect to the sample.

TEM studies [10, 11] unravel that in $\alpha_2$-Ti$_3$Al, the (0001) basal, and $\{10\bar{1}1\}$, $\{10\bar{1}2\}$, and $\{10\bar{1}3\}$ pyramidal planes are the habit planes for cleavage fracture. However, the effect of crystallographic orientation on crack propagation mechanisms in $\alpha_2$-Ti$_3$Al has not been investigated yet.

The most straightforward relationships between material parameters and the fracture toughness of an alloy are given by the criteria of Griffith for cleavage [12] and of Rice for dislocation emission [13, 14] at the crack tip, derived from continuum elasticity considerations. Details are given in section 2.1. Based on the critical stress intensity factors (SIF) $K_c$ for cleavage, respectively $K_R$ for dislocation emission, the crack tip mechanism can be predicted. E.g., if $K_c < K_R$ for a particular crack system, brittle cleavage is energetically more favorable than dislocation emission at the crack tip. However, the reliability of this theoretical prediction of the crack tip mechanism based on anisotropic linear elastic fracture mechanics (ALEFM) has not yet been proven for Ti-Al alloys. Since the actual atomistic mechanisms that occur at the crack tip are influenced by several factors, such as surface stress distribution due to the initial crack, the
crack tip geometry, the local composition of the cleavage surfaces, etc, this cannot be done analytically. Therefore, we perform embedded atom method (EAM) based molecular statics (MS) simulations to verify the ALEFM predictions, and also to understand detailed atomistic level crack tip mechanisms. In this regard, it should be noted that the predictive capability of the Griffith or Rice criterion in determining crack tip mechanism requires the comprehensibility of the calculated free surface energies as well as the identification and analysis of all available dislocation slip systems and their associated stacking fault energies. In contrast, fcc metals have only one type of dominant slip system. Evaluation of the theoretical Griffith and Rice criteria thus predicts the crack tip behavior in close agreement with atomistic simulations as well as experiments [15, 16]. However, deviations can occur due to lattice trapping effects, which require an extension of the Rice criterion [17]. Bcc and hcp metals, for instance iron (Fe) and magnesium (Mg), on top of that, have multiple slip systems and exhibit complex dislocation core structures [18]. Furthermore, they have more than one possible type of cleavage plane.

Therefore, the goal of this paper is two-fold: to identify the atomistic crack tip mechanisms in Ti-Al depending on orientation and to evaluate the predictive capability of the continuum ALEFM criteria.

As will be seen in the following, we find good agreement between ALEFM and atomistic simulation predicted crack tip mechanisms, as long as the competing mechanisms are direct cleavage or dislocation emission. However, we observe additional crack tip mechanisms in both γ and α2 phase. The implications will be discussed.

The remainder of the paper is organized as follows. A detailed introduction into ALEFM based fracture criteria and to the atomistic simulation methodology is given in section 2. Crack tip events and associated mechanisms are analyzed in section 3, while conclusions are drawn in section 4.

2. Simulation method

2.1. Anisotropic linear elastic fracture mechanics: Griffith and Rice criterion

The well-known Griffith’s criterion for cleavage fracture [12] states that a crack propagates under mode-I loading if the energy release rate ($G_I$) exceeds the energy of the newly created surfaces, $2\gamma_s$. Thus, the critical energy release rate is

$$G_{IC} = 2\gamma_s.$$

The critical SIF under mode-I loading ($K_{IC}$) is proportional to $\sqrt{G_{IC}}$ [19]. Considering plane strain condition in an isotropic elastic media, this relation can be expressed as,

$$K_{IG} = \frac{E}{(1-\nu^2)} G_{IC},$$

where ‘$E$’ and ‘$\nu$’ are Young’s modulus and Poisson’s ratio. In case of full anisotropic elasticity, the energy release rate becomes

$$G = K^T \Lambda K$$

where $\Lambda$ is the Stroh energy tensor [20]. $K = [K_{II}, K_{I}, K_{III}]^T$ is the applied SIF for mixed mode loading. The Stroh energy tensor can be evaluated as

$$\Lambda = \frac{1}{2} \text{Re}(iAB^{-1})$$
where $A$ and $B$ are the eigenvectors evaluated as solution to the eigenvalue equation,

$$\mathbf{N} \begin{bmatrix} A \\ B \end{bmatrix} = \lambda \begin{bmatrix} A \\ B \end{bmatrix}.$$  \hfill (5)

$\mathbf{N}$ is the fundamental elasticity matrix [21], and can be written as

$$\mathbf{N} = \begin{bmatrix} \mathbf{N}_1 & \mathbf{N}_2 \\ \mathbf{N}_3 & \mathbf{N}_1^T \end{bmatrix}$$  \hfill (6)

with

$$\mathbf{N}_1 = -\mathbf{T}^{-1} \mathbf{R}^T, \quad \mathbf{N}_2 = \mathbf{T}^{-1}, \quad \mathbf{N}_3 = \mathbf{R} \mathbf{T}^{-1} \mathbf{R}^T - \mathbf{Q}$$  \hfill (7)

where

$$\mathbf{Q} = \begin{bmatrix} C_{11} & C_{16} & C_{15} \\ C_{16} & C_{66} & C_{56} \\ C_{15} & C_{56} & C_{55} \end{bmatrix}, \quad \mathbf{R} = \begin{bmatrix} C_{16} & C_{12} & C_{14} \\ C_{66} & C_{26} & C_{46} \\ C_{56} & C_{25} & C_{45} \end{bmatrix}$$  \hfill (8)

and

$$\mathbf{T} = \begin{bmatrix} C_{66} & C_{26} & C_{46} \\ C_{26} & C_{22} & C_{24} \\ C_{46} & C_{24} & C_{44} \end{bmatrix}.$$  \hfill (9)

$C_{ij}$ in the above equations are the elements of the material stiffness tensor under Voigt notation. For anisotropic elasticity and plane strain conditions, $K_{IC}^G$ for pure mode-I loading can be evaluated as [22],

$$K_{IC}^G = \sqrt{\frac{2}{\Lambda_{22}}} \gamma_s \Lambda_{22}^2.$$  \hfill (10)

To take into account crack tip plasticity, Rice’s criterion [13] considers the contribution of the unstable stacking fault energy ($\gamma_{usf}$) as the barrier for dislocation emission. Different potential slip planes, oriented obliquely with respect to the crack system, have to be evaluated to determine the one with the lowest critical SIF. Under mode-I loading and plane strain conditions, $(K_{IC}^R)$ of an isotropic elastic material then can be expressed as [22],

$$K_{IC}^R = \sqrt{\frac{16\mu(1 + (1 - \nu)\tan^2\phi)}{(1 - \nu)(1 + \cos\theta)\sin^2\theta \gamma_{usf}}} \gamma_{usf}$$  \hfill (11)

where $\theta$ and $\phi$ are the angle between crack direction and slip plane, and crack plane and Burgers vector. Considering anisotropy, equation (11) can be written as [14],

$$K_{IC}^R = \sqrt{\frac{16\mu(1 + (1 - \nu)\tan^2\phi)}{(1 - \nu)(1 + \cos\theta)\sin^2\theta \gamma_{usf}}} \gamma_{usf} \zeta(\theta, \phi)$$  \hfill (12)

where $\zeta(\theta, \phi)$ is the elastic property for shear along the slip direction, and is given by

$$\zeta(\theta, \phi) = b(\phi)A_{ij}^{(\theta)} b(\phi)$$  \hfill (13)

with

$$b(\phi) = (\cos\theta, 0, \sin\phi).$$  \hfill (14)
\( \mathbf{b} \) is the slip vector of the dislocation emitted at the crack tip and \( \Lambda_{ij}^{(\theta)} \) is the rotated Stroh energy density tensor \([20]\),

\[
\Lambda_{ij}^{(\theta)} = \Omega_{ik} \Lambda_{kl} \Omega_{jl}
\]  

(15)

where \( \Omega \) is the rotation matrix given by

\[
\Omega = \begin{bmatrix}
\cos \theta & \sin \theta & 0 \\
-\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{bmatrix}.
\]  

(16)

More detailed theoretical descriptions of fracture, and the Griffith and Rice criteria within ALEFM can be found in references \([18, 20, 22]\).

The required material parameters of \( \gamma \) and \( \alpha_2\)-TiAl such as elastic constants \( (C_{ij}) \), surface energy \( (\gamma_s) \), and unstable stacking fault energy \( (\gamma_{usf}) \) are calculated directly from the EAM potential \([25]\) that we employ for our atomistic simulations, see table 1. These calculated parameters are consistent with the parameters used for fitting in the EAM potential \([25]\). The EAM potential for TiAl developed by Zope \( \text{et al.} [25] \) is widely used to describe fracture and deformation in TiAl \([26–28]\), since it reproduces the material parameters that determine the fracture behavior reasonably well, when compared to experimental values \([23, 24]\), as can be seen in table 1. The calculated values are used in equations (10) and (12) to predict the crack tip mechanism. In order to evaluate the predictive capability of ALEFM and to understand the atomistic mechanisms of the crack tip behavior, we perform MS simulations as described in the next section.

### 2.2. Atomistic simulation method

All the atomistic simulations are carried out using the large-scale atomic/molecular massively parallel simulator \([29]\) with the EAM potential of Zope \([25]\) mentioned above. For visualization, the open visualization tool OVITO \([30]\) is used.

We first generate single crystal configurations of face centered tetragonal \( \gamma \) and hexagonal closed pack \( \alpha_2\)-TiAl such that the desired crack propagation direction is oriented along the \( X \) axis, while the other two orthogonal directions are lying along the \( Y \) and \( Z \) axis, respectively. The crack systems studied in this work are listed in table 2. Due to the tetragonality of \( \gamma\)-TiAl (\( \delta = 1.047 \)), the \( c \)-direction is not equivalent to the \( a \) and \( b \) directions, as it would be the case in a cubic structure. Therefore, we use a notation with mixed parentheses \([31]\), \( \langleuvw\rangle \) and \( \{hkl\} \) to indicate that the first two indices can be permuted or can change sign, but the third one is fixed.

To eliminate any residual stress generated due to lattice rotation, the initial configurations are minimized using the conjugate gradient method with a force tolerance limit of \( 10^{-15} \text{eV Å}^{-1} \).

An atomistically sharp and semi-infinite crack is inserted in the relaxed configuration of the initial samples by displacing the atoms according to the linear-elastic solution around the crack tip considering plane strain condition in an anisotropic body \([32]\) for mode-I loading. The anisotropic displacement field near the crack tip is briefly discussed in appendix A of this paper. To maintain a plane strain condition, periodic boundary conditions are imposed along the \( Z \) direction. A representative initial simulation set-up is shown in figure 1. This simulation set-up is commonly known as \( K \)-test geometry and has already been successfully applied in numerous studies \([18, 22, 33, 34]\). Note, however, that quasi-static loading prevents symmetry-breaking operations such as those enabled by thermal fluctuations at finite temperatures in
Table 1. Material parameters of single phase $\gamma$ and $\alpha_2$-TiAl as obtained from EAM potential for TiAl [25]. Elastic constants of $\gamma$ and $\alpha_2$-TiAl are compared with previous experiments by Tanaka et al [24], and Watson et al [24], respectively.

| Structures | Elastic constants (GPa) | Surface energy ($\gamma_s$) (mJ m$^{-2}$) | Unstable stacking fault energy ($\gamma_{usf}$) (mJ m$^{-2}$) |
|------------|-------------------------|------------------------------------------|-------------------------------------------------|
| $\gamma$-TiAl | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{33}$ | $C_{44}$ | $C_{66}$ | (100) plane | (111) plane | (110) plane | (111) plane | (110) plane |
| This work  | 195  | 107  | 113  | 213  | 92  | 84  | 1177 | 212 {111}(112) | 1445 {110} |
| Expt. [23] | 183  | 74.1 | 74.4 | 178  | 105 | 78.4 | 1145 | 426 {111}(110) | 535 {110} |
| $\alpha_2$-Ti3Al | This work | 180  | 74   | 70   | 223 | 47  | 127 | 1748 (1010) | 576 (0001) [1120]-basal |
| Expt. [24] | 175  | 88.7 | 62.3 | 220  | 62.2| 131.85 | 1247 (0001) | 665 (1100)[1120]-prismatic |
|             |            |      |      |      | 671 (1121)[1126]-pyramidal |
Table 2. List of different crack systems studied in this work.

| Crack orientations                      | γ-TiAl | α2-Ti3Al |
|-----------------------------------------|--------|----------|
| {010}<100>                             |        |          |
| {110}<110>                             |        |          |
| {110}<111>                             | (010)<1210> |        |
| {110}<110>                             | (1210)<1010> |      |
| {111}<110>                             | (0001)<1210> |      |
| {111}<112>                             |        | (1010)<0001> |
| {111}<211>                             |        |          |

Figure 1. Simulation set-up. As denoted in the figure, X and Y axes are oriented along crack propagation direction and normal to the crack plane, respectively.

real samples, and therefore $K_{IC}$ values determined during quasi-static loading are likely to be somewhat overestimated.

To find the atomistically sharp but stable configuration of the initial crack, we open the initial crack using a SIF value ($K_{IC}^{at}$) which is quite close to the predicted lowest $K_{IC}^{G}$ or $K_{IC}^{R}$ value of that particular crack system. We relax the system keeping the atoms outside the cylindrical region fixed, see figure 1. We observe that the crack tips are stable for $K_{IC}^{at} \approx 0.90–0.95 \min\{K_{IC}^{G}, K_{IC}^{R}\}$ depending on crack orientation. The system containing the initial stable crack is further loaded by applying the same anisotropic displacement field [32] (appendix A) in a quasi-static manner. The $K_{IC}^{at}$ value is increased by $\sim 1\%$ of the $\min\{K_{IC}^{G}, K_{IC}^{R}\}$ for that particular crack orientation in each step, followed by energy relaxation. The crack tip location is tracked based on energy and on pairwise distance of the atoms at the tip. The position of the atom with the highest energy at the tip is considered as the new crack tip location, and this instantaneous crack tip position is used as new origin to impose the displacement boundary conditions in the next loading step. The crack tip identification method is further illustrated in appendix B.

We investigate the effect of simulation cell size on $K_{IC}^{at}$ and on the crack tip phenomenon in order to eliminate any finite size effect. Figure 2 shows the effect of the $L_x$ and $L_y$ dimension on $K_{IC}^{at}$. The minimum cell dimensions for reasonable convergence of $K_{IC}^{at}$ are $L_x = L_y = 70$ nm.
Figure 2. Calculated $K_{IC}$ values of (010)[100] crack in $\gamma$-TiAl for different simulation cell size. The horizontal blue line indicates the ALEFM predicted critical SIF of brittle cleavage, $K_{IC}^c$.

This implies that to get a converged $K_{IC}$ value in TiAl, the crack tip should be placed at least 35 nm away from the boundary so that the fracture process zone [22] is not influenced by the far field stress. The simulation cell dimension along the $Z$ axis ($L_z$) has to be large enough to allow dislocation nucleation for oblique slip systems [9, 18]. To investigate the effect of $L_z$ on crack tip mechanism, we carried out simulations with varying $L_z$ from $L_z = 5$ nm up to 25 nm, but do not find any change in $K_{IC}^{c}$ value as well as in the crack tip mechanisms. Thus, $L_z \approx 10 \times r_c \approx 5$ nm ($r_c = $ interaction cut-off as defined in the EAM potential) is sufficient to facilitate oblique slip systems to get activated during loading. However, in our study we conduct large-scale simulation using the box dimension of $L_x = L_y = 100$ nm, and $L_z = 5$ nm, which is larger than the minimum cell dimension required for convergence.

3. Results and discussion

3.1. Crack tip mechanism in $\gamma$-TiAl

3.1.1. Validation of ALEFM predictions. The critical SIF values are calculated for all the crack systems using Griffith’s ($K_{IC}^{G}$) and Rice’s ($K_{IC}^{R}$) criterion (equations (10) and (12)) under the framework of ALEFM. In case of Rice, we have calculated $K_{1}$ values for all available slip systems in $\gamma$-TiAl, and the lowest one is considered as the critical SIF ($K_{IC}^{R}$) required for dislocation emission at the crack tip. The critical $K_{IC}^{R}$ values, $K_{IC}^{c}$, are also determined directly from our MS simulations. A comparison among the $K_{IC}$ values as obtained from ALEFM and MS simulations is made in figure 3. Figure 4 shows the cross-sectional view of the crack tip region perpendicular to the crack line at different external load ($K_{IC}^{R}$ values) for all the crack systems considered in $\gamma$-TiAl, table 2.

A comparison between ALEFM predicted $K_{IC}^{G}$ and $K_{IC}^{R}$ values for individual crack systems in $\gamma$-TiAl shows that crack systems [010][100], [110][110] and [110][111] are predicted to fail via cleavage ($K_{IC}^{G} < K_{IC}^{R}$), emission of a dislocation ($K_{IC}^{R} < K_{IC}^{G}$) and cleavage ($K_{IC}^{R} < K_{IC}^{G}$), respectively (figures 3(a)–(c)). Figures 4(a)–(c) show that this is in agreement with the atomistic mechanisms observed in our MS simulations. Especially cracks along [100] and [111] on crack plane [010] and [110] exhibit considerable crack tip advancement through sequential bond breaking at the crack tip, therefore, demonstrate brittle cleavage as depicted in figures 4(a) and (c). Cracks on the [111] plane propagating along different directions such...
Figure 3. Comparison of calculated critical stress intensities using atomistic simulations ($K_{IC}^a$), Griffith’s criterion ($K_{IC}^G$), and Rice’s criterion ($K_{IC}^R$), for different crack systems in $\gamma$-TiAl, as shown schematically in the figure. Crack tip mechanisms as observed in atomistic simulations are denoted with c for cleavage and e for dislocation emission.

Figure 4. View perpendicular to the crack front of the relaxed atomic configurations of the crack tip region at different $K_{IC}$ values for crack systems in $\gamma$-TiAl. Ti atoms are represented by bigger, Al atoms by smaller balls. Atoms are colored based on their local lattice structure by using adaptive common neighbor analysis.

Cracks on the $\{111\}$ plane exhibit the lowest value of $K_{IC}$ while $\{110\}$-cracks possess the highest one, in accordance with their surface ($\gamma_s$) and unstable stacking fault energies ($\gamma_{usf}$), table 1. This qualitative ordering of $K_{IC}^G$ or $K_{IC}^R$ values as obtained from continuum based
ALEFM calculation and our MS simulations is consistent with previous DFT results [8]. Moreover, it is now apparent that the effect of anisotropy on crack tip mechanism in γ-TiAl is quite pronounced, not only for cracks on a {110} plane, but also for {111} cracks.

3.1.2. Quantitative evaluation of the critical SIF. The min{\(K_{IC}^G, K_{IC}^R\)} values show a good quantitative agreement with the MS values. The exception is crack system \(\{010\} \langle 100 \rangle\), which fails by cleavage with a significantly higher \(K_{IC}^G\) than the predicted \(K_{IC}^R\). This could be attributed to the lattice trapping effect, caused by the discreteness of the crystal lattice (e.g. [35]), respectively due to quasi-static loading, which is likely to somewhat overestimate the \(K_{IC}\) value. Other than that no appreciable lattice trapping is observed in the crack systems investigated in our study.

An advantage of the continuum perspective on fracture is that we can evaluate the SIF for both potential mechanisms, and thus estimate how likely a change in mechanism can occur. Figure 3 illustrates that there is a significant difference (\(\sim 15–25\%\)) between \(K_{IC}^G\) and \(K_{IC}^R\) values for most of the crack orientations. For instance, a crack along \(\langle 100 \rangle\) in the \{100\} plane has \(K_{IC}^G \approx 0.64\) MPa\(\sqrt{m}\) while \(K_{IC}^R \approx 0.80\) MPa\(\sqrt{m}\), therefore, \(K_{IC}^G < K_{IC}^R\). For this particular orientation of crack, brittle fracture through cleavage, is significantly more favorable and expected to be a robust mechanism. Similarly, dislocation emission from the crack tip is by far more favorable than direct cleavage for crack propagation along \(\langle 110 \rangle\) in \{111\} plane.

In contrast, for the \{110\} \langle 110 \rangle and \{111\} \langle 110 \rangle crack systems \(K_{IC}^G\) and \(K_{IC}^R\) differ by only roughly 0.04 MPa\(\sqrt{m}\), indicating a close competition between dislocation emission and cleavage. A change in stacking fault energy due to alloying or a super-imposed stress state could cause a change in mechanism. Furthermore, deviations of the material parameters predicted by the potential compared to the experimental ones make a definitive prediction of crack tip mechanism in these crack systems difficult (even if our study is consistent in the sense that the same potential has been used for continuum and MS studies).

3.1.3. Analysis of crack tip mechanisms. Next, we describe the crack tip mechanisms for the individual crack systems considered in this study. For the crack system \(\{010\} \langle 100 \rangle\), ideal brittle crack propagation is predicted (figure 3). Brittle fracture in the \{010\} plane was also observed experimentally [4]. Consistent with these observations and predictions, we observe sequential bond breaking at the crack tip which leads to brittle crack propagation in \(\{010\} \langle 100 \rangle\), as shown in figure 4(a): the crack tip maintains atomistically sharp geometry even at a higher load. It is worth noting that the crack is observed to be closed at \(K_{IC}\) values lower than \(K_{IC}^G\) or \(K_{IC}^R\), and a stable configuration is obtained at \(K_{IC} = 0.97\) \(K_{IC}^G\) or \(K_{IC}^R\). Upon further loading, the opening stress \(\sigma_{yy}\) is observed to accumulate at the crack tip and crack propagation is initiated at \(\sigma_{yy} \approx 15–16\) GPa, without showing any plastic deformation.

According to the ALEFM criteria, the crack system \(\{110\} \langle 110 \rangle\) is predicted to emit a dislocation (figure 3(b)). The Rice value in figure 3(b) is the result of equation (12) for slip system \(\frac{1}{2}\langle 110 \rangle\{110\}. The existence of this special dislocation (not ordinary slip) in γ-TiAl was first reported by Panova et al [9]. As a consequence, the crack along \(\langle 110 \rangle\) in \{110\} plane shows no considerable propagation, but the crack tip exhibits blunting even at a higher value of \(K_{IC}\) (figure 4(b)). Ultimately, at an opening stress \(\sigma_{yy}\) of \(\sim 9.5\) GPa (\(K_{IC}^G = K_{IC}^R\)), a perfect dislocation is emitted from the crack tip as is predicted by ALEFM. Upon emission, this dislocation rapidly starts gliding on \{110\}, and either sides of the crack plane show a rigid shift like displacement parallel to the \{110\} plane, which creates a new \{110\} surface. Thus, crack propagation along \(\langle 110 \rangle\) in the \{110\} plane is impeded by plastic deformation (dislocation emission). In contrast, a crack in the same \{110\} plane propagates by cleavage along \{111\}. The \(K_{IC}^G\) value for crack along \{111\} is slightly higher compared to crack along \(\langle 110 \rangle\) on the same \{110\} plane.
Figure 5. Comparison of calculated critical stress intensities using atomistic simulations ($K_{\text{at}}^I$), Griffith criterion ($K_{\text{G}}^I$), and Rice criterion ($K_{\text{R}}^I$), for different crack systems in $\alpha_2$-TiAl, as shown schematically in the figure. Crack tip mechanisms as observed in atomistic simulations are denoted with c for brittle cleavage and e for dislocation emission.

For the crack plane $\{111\}$, we examined three different crack propagation directions, $\langle110\rangle$, $\langle112\rangle$, and $\langle211\rangle$. Among them, the first two crack orientations are potential ordinary slip and twinning systems in $\gamma$-TiAl. Indeed, dislocation emission for these crack orientations is predicted by ALEFM (figures 3(d) and (e)). In accordance with their difference in $\gamma_{\text{usf}}$ values for slip along $\langle110\rangle$ and $\langle112\rangle$, crack orientation $\{111\}\langle110\rangle$ exhibits a larger $K_{\text{R}}^I$ value than $\{111\}\langle112\rangle$, as shown in figure 3. Nevertheless, in both cases, upon loading, the crack tip emits Shockley type partial (twinning) dislocations with Burgers vectors $\langle1\bar{1}2\rangle$ (figures 4(d) and (e)). Instead of crack propagation, crack tip blunting occurs due to glide of the partials, which leave behind superlattice intrinsic stacking faults (SISF), the energetically most favorable faults in $\gamma$-TiAl. Consequently, a large free surface is created just ahead of the initial crack tip. In sharp contrast, a crack in the same $\{111\}$ plane but propagating along $\langle211\rangle$ shows clear brittle cleavage maintaining an atomistically sharp geometry of the crack tip.

This directional dependence of the crack tip mechanism in the $\{111\}$ plane is another striking manifestation of the anisotropy of fracture in $\gamma$-TiAl.

### 3.2. Crack tip mechanism in $\alpha_2$-Ti$_3$Al

#### 3.2.1. Validation of ALEFM predictions.  
ALEFM predicted critical stress intensities are compared with those obtained directly from our atomistic simulations ($K_{\text{at}}^I$) in figure 5. Figures 6 and 7 show the cross-section of the atomistic sample with prismatic cracks $\langle10\bar{1}\rangle[1\bar{2}1\bar{0}]$ and $\langle1\bar{2}1\rangle[1\bar{0}1\bar{0}]$, and basal crack systems $\langle0001\rangle[1\bar{2}1\bar{0}]$ and $\langle0001\rangle[10\bar{1}0]$, respectively, in a plane perpendicular to the crack tip direction at different applied $K_I$ values. In the inset of figures 6 and 7, crack tip regions and dislocations (if any) are shown.

As depicted in figures 5(a)–(c), for both the prismatic cracks, $\langle10\bar{1}\rangle[1210]$ and $\langle1\bar{2}1\rangle[1010]$, and for the first basal crack $\langle0001\rangle[1210]$, $K_{\text{G}}^I$ is always lower than $K_{\text{R}}^I$, the differences being $\sim$20–50%. Therefore, all of these cracks should be prone to brittle cleavage. Indeed, in our atomistic simulations, we observe crack tip advancement by bond breaking at the crack tip for these systems, see figures 6(a)–(d) and (e)–(h) ($\langle10\bar{1}\rangle[1210]$ and $\langle1\bar{2}1\rangle[1010]$) and figures 7(a)–(d) ($\langle0001\rangle[1210]$).

However, emission of dislocations is observed at higher applied loads for both the prismatic crack systems, which makes the identification of the crack tip mechanism via the Griffith and Rice criteria unreliable. A more detailed discussion follows in section 3.2.3.
In contrast, nucleation of a pyramidal II type dislocation \( \frac{1}{4}[12\overline{1}6][12\overline{1}] \) is predicted for the basal crack propagating along \([10\overline{1}0]\): \( K_R^{IC} = 0.76 \text{ MPa}\sqrt{m} \), while \( K_G^{IC} \) is slightly higher, 0.79 MPa\(\sqrt{m} \), see figure 5(d). Our atomistic simulation indeed shows onset of shear along \([12\overline{1}1]\) at a stress intensity slightly higher than \( K_R^{IC} \), followed by crack blunting, figures 7(e)–(h). However, this shear instability is not characterised by any lattice Burgers vector of the \( \alpha_2 \) structure.

3.2.2. Quantitative evaluation of the critical SIF. The critical stress intensities obtained from the atomistic simulations (\( K_{IC}^{at} \)) are very close to the ALEFM predicted \( K_{IC}^{A} \) or \( K_{IC}^{G} \) values for all crack systems. Crack system (0001)[10\overline{1}0] also exhibits very close ALEFM based values for \( K_{IC}^{G} \) and \( K_{IC}^{R} \), \( K_{IC}^{G} = 0.79 \text{ MPa}\sqrt{m} \), and \( K_{IC}^{R} = 0.76 \text{ MPa}\sqrt{m} \), see figure 5(d), indicating that the mechanism is prone to changes (compare discussion in section 3.1.2).

Figure 5 illustrates that the basal cracks (0001)[12\overline{1}0] and (0001)[10\overline{1}0] possess the lowest values of \( K_I \). This is because of the substantially lower surface energy (1247.42 mJ m\(^{-2}\)) and effective shear modulus (\( C_{44} = 46.6 \text{ GPa} \)) of the (0001) basal plane as compared with prismatic planes (10\overline{1}0) and (12\overline{1}0) in \( \alpha_2 \)-TiAl, see table 1). This is also well consistent with the results of TEM studies [5–7], in which basal planes are observed as the habit plane for crack growth in \( \alpha_2 \)-TiAl.

In general, all critical \( K_{IC} \) values in \( \alpha_2 \)-TiAl are higher than those in \( \gamma \)-TiAl, even those of the basal plane, in agreement with the experimental experience that the \( \alpha_2 \) phase generally has the higher fracture toughness and can arrest cracks in two-phase lamellar TiAl structures.

3.2.3. Analysis of crack tip mechanisms. Our atomistic simulations show that for the prismatic crack system (10\overline{1}0)[12\overline{1}0] the crack tip starts propagating by direct bond breaking.
maintaining the geometry of the atomically sharp crack, as shown in figures 6(a) and (b). The two consecutive pair of neighboring atoms, Ti–Al and Al–Al, are observed to separate as indicated by black balls and sticks in the inset of figures 6(a) and (b). After relaxation, their pair-distance exceeds ~192% of the equilibrium first nearest neighbor distance of α2-Ti3Al which indicates clear bond breaking. Up to this point, the prediction of cleavage via the Griffith criterion is correct, which explains the quantitative agreement between $K_{at}$ and $K_G$. However, upon further loading above $K_{at}$, typically at $K_{at}^c = 1.125 K_{atc}$, the crack tip shows complete blunting, and consequently, it emits a prismatic dislocation $\frac{1}{2}[1210](1100)$, figure 6(c). At higher values of $K_{at}$, until $K_{at}^c \approx 1.27 K_{atc}$, the dislocation keeps on gliding towards the surface of the sample and at $K_{at}^c = 1.28 K_{atc}$, another prismatic dislocation $\frac{1}{2}[1210](0110)$ is emitted on the conjugate prismatic plane as shown in figure 6(d). Eventually, the crack is observed to be blunted through dislocation mediated plastic deformation while the crack tip attains an arrow like shape where two conjugate prismatic planes are arranged obliquely, figure 6(d).

Similarly, the other prismatic crack (1210)[1010] is also predicted to show brittle cleavage by ALEFM, figure 5(b). The difference between the two prismatic cracks is the atomic arrangement of Ti and Al atoms in the crack planes. In the latter case, for crack system (1210)[1010], the two sides of the crack planes are not smooth on the atomic scale, and as a result, the initial crack tip geometry is not atomically sharp, but slightly wavy. A similar kind of bond breaking as before is observed at $K_{at}^c = 1.0 K_{atc}$, see the insets of figures 6(e) and (f). Subsequently, the crack tip is observed to propagate ~10 Å, before nucleating a prismatic dislocation $\frac{1}{2}[1210](1010)$ at $K_{at}^c = 1.14 K_{atc}$, figure 6(g). Upon further loading two more prismatic dislocations, $\frac{1}{2}[1210](1010)$ and $\frac{1}{2}[1210](1100)$, are emitted from the crack tip leading to crack blunting, figure 6(h). The first event through which crack propagation initiates for the crack
system (1210)[1010] is brittle cleavage, which is also consistent with prior ALEFM prediction, see figure 5(b).

Thus, so far we observe that the very first atomic event that takes place at the crack tip for both the prismatic crack systems (1010)[1210] and (1210)[1010] is cleavage, which is consistent with the ALEFM prediction. However, at higher values of $K_I$ the crack tip mechanisms change. To confirm that the initial displacement of the crack tip is not a finite size effect [22] we perform simulations with $L_x = L_y$ up to 200 nm, but the observed type of mixed mechanism persists. It can be understood by calculating the theoretical opening stress ($\sigma_{yy}^{th}$) and shear stress ($\sigma_{xy}^{th}$) within an ALEFM framework using equations (A.2) and (A.3), appendix A, for given $K_I$ values. For the crack system (1010)[1210], at $K_I^{th} = 1.0 K_{Ic}^{th}$, $\sigma_{yy}^{th} = 14.56$ GPa and $\sigma_{xy}^{th} = 8.47$ GPa, while the atomistically obtained values are $\sigma_{yy}^{at} = 18.76$ GPa and $\sigma_{xy}^{at} = 15.12$ GPa, respectively. This means that in the atomistic simulations the shear stress ($\sigma_{xy}^{at}$) developed at the crack tip is almost twice the theoretically predicted one.

Eventually, this results in prismatic slip which is also predicted by Rice i.e., $K_I^{th}(1\overline{2}10)(10\overline{1}0) = 6.973$ MPa/\(\sqrt{m}\), see figure 5(a). A similarly high shear stress state occurs in the crack system (1210)[1010] and consequently dislocation mediated plasticity is observed there, too, followed by crack blunting.

Consistent with previous TEM reports and the ALEFM prediction, we observe that a crack along [1\overline{2}10] on the (0001) basal plane propagates through direct bond breaking, i.e. cleavage, as shown in figures 7(a)–(d). The onset of crack propagation is identified at a very low opening stress ($\sigma_{yy} = 5.8$ GPa) compared to other crack systems in $\alpha_2$-Ti$_3$Al. Even at higher loads ($K_I^{at} \gg K_{Ic}^{at}$), no signature of plastic deformation is observed, rather, the crack tip maintains an atomically sharp geometry and advances via sequential bond breaking.

As mentioned above, for crack propagation direction [1010] in the basal plane, ALEFM predicts a close competition between brittle cleavage and the emission of a dislocation into the pyramidal II (1\overline{2}16)[1211]) slip system. In the atomistic simulations, a slip process along the pyramidal II slip plane is indeed observed, as shown in figure 7(f). However, the atomic disregistry along the fault line shows that the slip does not generate a dislocation core, but it causes a general shear instability. Upon further loading, another slip event on the conjugate pyramidal II plane, (1211), is observed, figure 7(h). The slip is mediated via a rigid sliding of neighboring half-crystals, with only some distortions of the atomistic structure directly at the slip plane. Such a rigid shear mechanism was also observed at the typical $\gamma/\gamma$ rotational boundaries in Ti–Al lamellar microstructures [28] under shear loading.

4. Summary and conclusions

We systematically investigate the crack tip mechanisms in anisotropic single crystal $\gamma$-TiAl and $\alpha_2$-Ti$_3$Al. For predictions of the crack propagation mechanisms, we use the so-called Rice and Griffith criteria, which can be derived from linear elastic fracture mechanics and augmented to take into account elastic anisotropy via the full tensor of elastic constants. We verify the predictions via EAM based MS simulations. The results provide new insights into the atomistic details and the orientation dependence of crack tip mechanisms in these systems, as well as on the applicability of continuum-elasticity based criteria to anisotropic, binary alloys.

In $\gamma$-TiAl, cracks in the {111} plane show the lowest fracture toughness while cracks in {110} possess the highest. Cracks on both planes exhibit either brittle cleavage or emission of dislocation, depending on the crack propagation direction.

$\alpha_2$-Ti$_3$Al generally exhibits higher critical $K_I$ values than $\gamma$-TiAl. Most of the crack systems (prismatic and basal) initially fail through cleavage, but at higher applied load they demonstrate crack blunting through local crack tip plasticity mediated by emission of dislocations. These
blunted cracks in α2-Ti3Al are also commonly observed in TEM experiments. The basal plane is generally assumed to be prone to brittle cleavage only, but we observe that it this not the case, rather the basal crack along [10\bar{1}0] shows crack blunting through a shear mechanism.

Our comparison to the predictions of LEFM reveals that the Griffith and Rice criteria can indeed determine the critical SIF and the possible cracktip mechanisms on the atomistic scale, if elastic anisotropy is taken into account and as long as the processes are limited to dislocation emission and brittle cleavage. For the proper application of the criteria, all the available dislocation slip systems and their respective stacking fault energies have to be known and evaluated. For crack blunting due to mixed mechanisms, or shear instabilities other than dislocation emission, one still obtains a reliable critical value for the SIF from ALEFM, but one has to look at the atomistic details to reliably identify the underlying mechanism.

Acknowledgments

This work was supported by the German Science Foundation (DFG) under grant number 404541620.

Appendix A. Anisotropic displacement field at crack tip for mode-I loading

Under the framework of anisotropic ALEFM, the stress field at the crack tip under mode-I loading can be expressed as,

\[ \sigma_{xx} = \frac{K_1}{\sqrt{2\pi r}} Re \left[ \frac{a_1 a_2}{a_1 - a_2} \left( \frac{a_2}{\sqrt{\cos \theta + a_2 \sin \theta}} - \frac{a_1}{\sqrt{\cos \theta + a_1 \sin \theta}} \right) \right] \]  
(A.1)

\[ \sigma_{yy} = \frac{K_1}{\sqrt{2\pi r}} Re \left[ \frac{1}{a_1 - a_2} \left( \frac{a_4}{\sqrt{\cos \theta + a_4 \sin \theta}} - \frac{a_2}{\sqrt{\cos \theta + a_2 \sin \theta}} \right) \right] \]  
(A.2)

\[ \sigma_{xy} = \frac{K_1}{\sqrt{2\pi r}} Re \left[ \frac{a_1 a_2}{a_1 - a_2} \left( \frac{1}{\sqrt{\cos \theta + a_1 \sin \theta}} - \frac{1}{\sqrt{\cos \theta + a_2 \sin \theta}} \right) \right] \]  
(A.3)

Accordingly, the displacement field near the crack tip can be expressed as,

\[ u_x = K_1 \sqrt{\frac{2r}{\pi}} Re \left[ \frac{1}{a_1 - a_2} \left( a_1 p_2 \sqrt{\cos \theta + a_2 \sin \theta} - a_2 p_1 \sqrt{\cos \theta + a_1 \sin \theta} \right) \right] \]  
(A.4)

\[ u_y = K_1 \sqrt{\frac{2r}{\pi}} Re \left[ \frac{1}{a_1 - a_2} \left( a_1 q_2 \sqrt{\cos \theta + a_2 \sin \theta} - a_2 q_1 \sqrt{\cos \theta + a_1 \sin \theta} \right) \right] \]  
(A.5)

where \((r, \theta)\) defines the position around the crack front. The constants \(p_1, p_2, q_1,\) and \(q_2\) can be obtained from the equations below,

\[ p_1 = S^p_{11} a_1^2 + S^p_{12} - S^p_{16} a_1 \]

\[ p_2 = S^p_{11} a_2^2 + S^p_{12} - S^p_{16} a_2 \]

\[ q_1 = S^p_{11} q_1 + S^p_{22} q_1 a_1 - S^p_{26} \]

\[ q_2 = S^p_{11} q_2 + S^p_{22} q_2 a_2 - S^p_{26} \]  
(A.6)
where $a_1$ and $a_2$ are roots of the characteristic equation,

$$S_{11}^p a^4 - 2S_{16}^p a^3 + (2S_{12}^p + S_{66}^p) a^2 - 2S_{26}^p a + S_{22}^p = 0$$

(A.7)

and $S_{ij}^p = S_{ij} - \frac{S_{3i}S_{3j}}{S_{33}}$, where $S_{ij}$ are the components of compliance tensor expressed in Voigt notation for plane strain condition.

**Appendix B. Identification of crack tip position and $K_{IC}$**

The method to identify the crack tip position is briefly explained here, using the example of crack system $\{010\} \langle \overline{1}00 \rangle$ of $\gamma$-TiAl. Figures B.1(a) and (b) show the change in the potential energy of the system, and the crack tip position with increasing applied loading ($K$ values). As can be observed from Figure B.1(a), the potential energy of the sample rises continuously with increasing applied load, until at the critical value of $K$, a discontinuity occurs. The transition from the stable to an unstable configuration of the crack tip is marked by the transition from the yellow to the red region in the diagram. The corresponding $K$ value ($K = 0.681$ MPa/√m, marked by black arrows in figures B.1(a) and (b)) is considered to be the critical SIF-$K_{IC}$. After each cycle of loading and relaxation, the energy of the atoms ahead of the crack tip are scanned to identify the atom which possesses the highest energy. This atomic position is considered as the new crack tip for next cycle of loading.

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