Supplementary Materials

Atomistic underpinnings for dislocation emission behaviors at the crack tips in FCC metals in light of thermo-kinetic synergy

Kunyu Zhang[1], Jinglian Du[1,*], Jianwei Xiao[2], Ziding Yang[1], Jiaqi Yang[1], Kexing Song[3], Feng Liu[1,4,*]

[1]State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, Shaanxi, China.
[2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, Liaoning, China.
[3]Henan Academy of Sciences, Zhengzhou 450046, Henan, China.
[4]Analytical & Testing Center, Northwestern Polytechnical University, Xi'an 710072, Shaanxi, China.

[*]**Correspondence to:** Prof. Jinglian Du, Prof. Feng Liu, State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, Shaanxi, China.
E-mail: dujl666@nwpu.edu.cn; liufeng@nwpu.edu.cn

This file includes:

- **Atomic displacement criteria for dislocation emission at the crack tips in FCC Al**

The defects formation and evolution during dislocation emission at the crack tips are dominated by the motion behaviors of atoms and/or atomic clusters. Thus, the critical conditions for dislocation emission at the crack tips in FCC Al can be determined from the variations of atomic displacement during dislocation emission at the crack tips. Herein the first structural unit for dislocation emission at the crack tips in FCC Al is defined as follows: (i) The two atoms overlapped between the SF zone formed by the first partial dislocation emission at the crack tips and the dislocation emission plane, are denoted as the atomic pair 1 and 1', see Figure 5A in the main text, and the according displacement difference between these two atoms under the Mode I loading conditions is denoted as $\Delta 1$; (ii) the two atoms adjacent to the atomic pair 1 and 1' along the [112] direction is denoted as the atomic pair 2 and 2', with the according displacement difference being denoted as $\Delta 2$. The critical values $\Delta 1_c$ and $\Delta 2_c$ for the displacement difference $\Delta 1$ and $\Delta 2$ before dislocation emission reflect the critical points of both dislocation propagation and structural unit instability of the crack tips. As such, the other atomic pairs and the according displacement difference can be defined analogously. All of these atomic pairs with respect to the first structural unit for dislocation emission at the crack tips collectively form the SF zone corresponding to the emission of the first partial dislocation.

Figure 5A in the main text shows the variations in atomic displacement of the first structural unit with respect to the stress intensity factor. When the first partial dislocation emitted at the crack tips, the displacement difference between 1 and 1' atoms increase from $\Delta 1 = 0.35b_p$ to $0.48b_p$, while that between 2 and 2' atoms increase from $\Delta 2 = 0.36b_p$ to $0.53b_p$. Apparently, the critical value $\Delta 1_c = 0.35b_p$ is smaller than $\Delta 2_c = 0.36b_p$. According to Curtin's theory[1], the value of $\Delta 1$ is always larger than that of $\Delta 2$, given that both the surface step energy and SF energy should be overcome for the increase of $\Delta 1$, while only the SF energy should be overcome for the increase of $\Delta 2$. Such contradiction derives from the increase of local stress near $\Delta 2$ induced by

the superposition between the dislocation stress field and the tip stress field. To this end, the displacement difference $\Delta 3$ between 3 and 3' atomic pair was obtained. The results show that when the first partial dislocation emitted from the crack tips in FCC Al, the according displacement increases from $\Delta 3 = 0.22b_p$ to $0.42b_p$, and the ratio of the critical displacement difference is $\Delta 1_c/\Delta 3_c = 0.64$, which is close to the ratio of $\Delta 2_c/\Delta 1_c \approx 0.7$ statistically obtained from Curtin theory[1]. Therefore, the critical conditions for the first partial dislocation nucleation at the crack tips in FCC Al can be expressed via the atomic displacement differences as: $\Delta 1_c = 0.35b_p$ and $\Delta 3_c = 0.22b_p$. Moreover, the 3 and 3' atomic pair is closest to the first partial dislocation at the crack tips, and the increment of according displacement difference $\Delta 3$ is $0.2b_p$, which is larger than $0.17b_p$ for the increment of $\Delta 2$. This signifies that the stress field at the crack tips in FCC Al exerts attractive interaction on those atoms near the dislocation.

Since the second partial dislocation nucleates at the adjacent slip plane of the first partial dislocation, the second structural unit with respect to the second partial dislocation at the crack tips requires to move one interplanar spacing of $(11\bar{1})$ plane toward the crack tips. The atoms overlapped between the corresponding SF zone and the dislocation emission plane are denoted as I and I' atomic pairs of the second structural unit, with the displacement difference being denoted as ΔI. Analogously, the II and II' atomic pairs, along with subsequent atomic pairs of the other structural unit can be defined as the same with those of the first structural unit. Figure 5B in the main text shows that when the second partial dislocation emitted from the crack tips in FCC Al, the displacement difference for the I and I' atomic pairs increases from $\Delta I = 0.21b_p$ to $1.04b_p$, and that for the II and II' atomic pairs increases from $\Delta II = 0.18b_p$ to $1.02b_p$. Apparently, the critical value for the displacement difference of the second structural unit, i.e., $\Delta I_c = 0.21b_p$ is smaller than that of the first structural unit, i.e., $\Delta 1_c = 0.35b_p$. This indicates that the nucleation rate of the second partial dislocation at the crack tips in FCC Al is faster than that of the first partial dislocation. However, when the second partial dislocation emitted at the crack tips, the increment of the displacement difference ΔI in the second structural unit is $0.83b_p$, which is considerably larger than

$0.13b_p$, i.e., the increment of the displacement difference $\Delta 1$ in the first structural unit. Thus, the energy required for emission of the second partial dislocation at the crack tips is higher than that of the first partial dislocation, given that the energy consumed at the crack tips is positively related to the increment of the displacement difference in atomic pairs at the crack tips. Figure 5C in the main text shows the variations in displacement differences Δi and Δii of atomic pairs in the third structural unit with increasing the stress intensity factor, the result of which is similar to that of the second structural unit, see Figure 5B in the main text.

When the third partial dislocation emitted at the crack tips in FCC Al, the displacement difference in the third structural unit increases considerably from Δi= $0.34b_p$ to $1.02b_p$ with an increment of $0.68b_p$, which is smaller than that of $0.83b_p$ for the displacement difference ΔI in the second structural unit. This indicates that the energy required to dissipate for emission of the third partial dislocation at the crack tips in FCC Al is lower than that of the second partial dislocation. The results are in accordance with those analyzed from the nucleation energy of the second and third partial dislocations of Section 3.1 in the main text, and thus confirms that during the twinning dislocation nucleation, it is easier for emission of the third partial dislocation at the crack tips in FCC Al than that of the second partial dislocation. However, the emission of the third partial dislocation at the crack tips in FCC Al lags behind that of the second partial dislocation, since the critical displacement difference of the third structural unit is larger than that of the second structural unit. The crack tips in FCC Al become no longer stable when emits the fourth partial dislocation, in which case the criterion for crack instability is no longer suitable to analyze from the atomic displacement differences, and this is beyond the scope of this work.

Each dislocation emission at the crack tips in FCC Al corresponds to different structural unit. In general, the emission of arbitrary partial dislocation at the crack tips can delay the emission of subsequent partial dislocations, and the underlying reason is attributed to the coordinative deformation among the different structural units for dislocation emission at the crack tips. For example, when the stress intensity factor at the crack tips is K_I= 0.281 MPa·$m^{1/2}$, the displacement difference Δ_1 between 1 and 1’

atomic pairs in the first structural unit increases instantly. With the expression ofΔ_1= δ_1'– δ_1, it turns out that during dislocation emission, the magnitude of displacement δ_1' for atom 1' is significantly larger than that for atom 1, i.e., δ_1, However, the atomic pairs of the first structural unit and the second structural unit share those atoms with larger displacement, which increases the corresponding δ_I in the second structural unit, thus reduces the displacement difference ΔI. Consequently, a larger stress intensity factor is required for the atomic displacement difference to reach its critical value, and thus delay emission of the second partial dislocation at the crack tips in FCC Al. Similarly, the dislocation emission at the crack tips in FCC Al can suppress the dislocation emission on the adjacent slip planes, which is behaved as the downward steps of the displacement difference between the various atomic pairs, see Figure 5A-C in the main text. Although the atomic displacement generated by the emission of the fourth partial dislocation cannot be directly obtained herein, when the stress intensity factor increases to K_I= 0.545 MPa·m$^{1/2}$, the fourth partial dislocation also exerts influences on the other structural units at the crack tips, particularly the first structural unit, which is the original crack tip. With the crack propagating forward, the original crack tip tears to open, resulting in an upward step appeared in the displacement difference of the atomic pair for the first structural unit after the crack becoming unstable, see Figure 5A in the main text.

In addition to using the atomic displacement difference of structural units for dislocation emission at the crack tips to assess the ease or difficulty of dislocation nucleation, the increment of the stress intensity factor for each dislocation emission can also be used to make the evaluation. As shown in Figure 5D of the main text, it is most difficulty for nucleation of the first partial dislocation, which can be emitted when the stress intensity factor increases to K_I= 0.282 MPa·m$^{1/2}$. As the applied load increases gradually, the interval of dislocation emission at the crack tips in FCC Al shortens. The interval between the stress intensity factor for emission of the first partial dislocation and the second partial dislocation is ΔK_I= 0.152 MPa·m$^{1/2}$, while that for emission of the second partial dislocation and the third partial dislocations is only ΔK_I= 0.048 MPa·m$^{1/2}$. The behind reason can be understood that under the same

mechanism of dislocation nucleation at the crack tips, the rate of dislocation nucleation can be enhanced by increasing the applied load continuously. However, the interval between the stress intensity factor for emission of the third partial dislocation and the fourth partial dislocation is 0.064 MPa·$m^{1/2}$, such abnormal increase is derived from the mechanisms transition for dislocation nucleation at the crack tips in FCC Al.

- **Details on calculating the potential barrier for dislocation nucleation at the crack tips in FCC Al**

According to the continuum mechanics model proposed by Andric and Curtin[1], the critical energy release rate G_{Ie} for emission of the first partial dislocation at the crack tips depends on both the surface energy γ_s and the unstable SF energy γ_{usf}, see Eq. (3) in the main text. In terms of FCC Al, the surface energy is γ_s= 0.871 J/m², and the unstable SF energy is γ_{usf}= 0.155 J/m², which corresponds to the first peak point of the generalized SF energy curve shown in Figure 8A of the main text. Thus, the critical energy release rate for the initial dislocation nucleation at the crack tips in FCC Al is G_{Ie} = 0.204 J/m². Similarly, the critical energy release rate G_{Ie} for emission of the back twinning dislocation at the crack tips (corresponding to the second and third partial dislocations) depends on the unstable twinning fault energy γ_{utf} and the intrinsic SF energy γ_{isf}[2], which correspond to the second peak point and the saddle point of the generalized SF energy curve, respectively. As shown in Figure 8A of the main text, γ_{utf} = 0.562 J/m² and γ_{isf} = 0.12 J/m² for FCC Al. Combined with Eq. (5) in the main text and the expression for critical stress intensity factor: $K_{Ie}=\sqrt{G_{Ie}p(\theta,\psi)}/F_{12}(\theta)$[3], the critical energy release rate for twinning dislocation emission at the crack tips in FCC Al is obtained as: G_{Ie} = 0.441 J/m². Considering that the surface steps have already formed during the back twinning dislocation nucleation stage, the critical energy release rate involved in the present work should include contribution from the surface step energy, the value of which increases to G_{Ie} = 0.645 J/m².

Accordingly, the potential barrier of dislocation nucleation (or the critical energy release rate) corresponding to different stages of dislocation emission at the crack tips in FCC Al can be obtained on the basis of Figure 8B in the main text as follows: (I) When the dislocation nucleated at the crack tips, it is required to overcome the formation energy of surface steps on the dislocation emission plane, the value of which is proportional to the surface energy γ_s. (II) When the dislocation nucleated on the slip plane near the crack tips, it is required to overcome the unstable twinning fault energy γ_{utf}. (III) When the dislocation nucleated within the SF zone (or at the SF marginality), it is required to overcome the energy difference between the unstable SF energy γ_{usf} (or unstable twinning fault energy γ_{utf}) and the intrinsic SF energy γ_{isf}. (IV) When the dislocation nucleated on the dislocation emission plane after crack propagation, it is required to overcome the crack surface energy. As such, the potential barrier for other prospective mechanisms of dislocation nucleation at the crack tips in FCC metals can be obtained via the different combinations of the above four nucleation mechanisms. For example, there are competitions between the back twinning dislocation nucleation mechanism and the trailing dislocation nucleation mechanism at the crack tips in FCC metals. The nucleation position of the trailing dislocation is on the same slip plane as the first partial dislocation at the crack tips, and thus cannot form the twinning zone, indicating that the according nucleation potential barrier is determined by the unstable SF energy γ_{usf}. Since the trailing dislocation nucleates on the SF zone generated by the first partial dislocation, the intrinsic SF energy offsets the nucleation potential barrier partially, and thus the potential barrier for trailing dislocation nucleation decreases to γ_{usf} - γ_{isf}. Meanwhile, the contribution from the step formation energy to the dislocation nucleation barrier should be considered given that the trailing dislocation nucleated at the crack tips. Based on Curtin's expression[2] for the critical energy release rate G_{Ie} of the trailing dislocation emission at the crack tips, i.e.,

$$\begin{cases} G_{Ie}=0.0725\gamma_s+0.5(\gamma_{usf}-\gamma_{isf}), \gamma_s>6.9(\gamma_{usf}-\gamma_{isf}) \\ G_{Ie}=\gamma_{usf}-\gamma_{isf}, \gamma_s<6.9(\gamma_{usf}-\gamma_{isf}) \end{cases} \quad \text{(S1)}$$

the reasonability for above analysis on the potential barrier of dislocation nucleation at the crack tips in FCC metals can be verified. According to Eq. (S1), the contribution from surface energy γ_s to the potential barrier of dislocation nucleation can be ignored when the value of γ_s is low. Based on the above analysis, the potential barrier of forward twinning dislocation can be obtained. Since the nucleation of forward twinning dislocation belongs to the scope of twinning nucleation, and the primary potential barrier to be overcome is γ_{utf}-γ_{ssf}. The distinction lies in the fact that nucleation of the forward twinning dislocation requires crack propagation, which is accompanied by the formation of two free surfaces. Therefore, the potential barrier for forward twinning dislocation can be approximated as: $G_{Ie}= \gamma_{utf} -\gamma_{isf} + 2\gamma_s$. Since the nucleation of the forward twinning dislocation occurs after that of the back twinning dislocation, the potential barrier for forward twinning dislocation should increase to G_{Ie}= 2.046 J/m². As such, the potential barrier corresponding to the different mechanisms of dislocation nucleation at the crack tips in FCC metals can be uniformly expressed as the linear combination of γ_{utf}, γ_{isf}, γ_{ssf}, and γ_s, which correspond to the critical energy release rate G_{Ie} (or nucleation potential barrier) at different stages of dislocation nucleation at the crack tips, as given by Eq. (7) in the main text, where the stage I, stage II, and stage III represents the initial crack-tip dislocation nucleation, the back twinning dislocation nucleation, and the forward twin dislocation nucleation, respectively. Accordingly, the dislocation nucleation mechanism throughout the entire process of dislocation emission at the crack tips in FCC metals can be obtained by analyzing the coefficient matrices in Eq. (7) in the main text.

Reference

[1] Andric, P.; Curtin, W. A. New Theory for Mode I Crack-Tip Dislocation Emission. *J. Mech. Phys. Solids* **2017**, *106*, 315–337. DOI: 10.1016/j.jmps.2017.06.006.

[2] Andric, P.; Curtin, W. A. New Theory for Crack-Tip Twinning in FCC Metals. *J. Mech. Phys. Solids* **2018**, *113*, 144–161. DOI: 10.1016/j.jmps.2018.01.016.

[3] Rice, J. R. Dislocation Nucleation from a Crack Tip: An Analysis Based on the Peierls Concept. *J. Mech. Phys. Solids* **1992**, *40* (2), 239–271. DOI: 10.1016/S0022-5096(05)80012-2.