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Strong Crack Blunting by Hierarchical Nanotwins in Ultrafine/Nano-grained Metals

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A theoretical model is proposed to illustrate the effect of detwinning of the secondary twin lamellae on the emission of lattice dislocations from a semi-infinite crack tip in a hierarchically nanotwinned metal. The results obtained show that the potential of the crack tip to emit dislocations can be optimized and greatly enhanced by tuning the secondary twin spacing, which leads to strong crack blunting. Moreover, the hierarchical structure is able to produce significant toughening at very thin secondary twin lamellae, as observed in molecular dynamics simulations. As a result, the proposed model suggests a novel toughening mechanism in ultrafine/nano-grained metals.

Keywords: Hierarchical Nanotwins, Detwinning, Twin Boundary Migration, Dislocation Emission, Cracks

Hierarchical and gradient structures are ubiquitous in the biological world, such as Geckos' toe,[1] bone and bamboo.[2] The sophisticated structures formed in the natural selection process render the animals and plants an extraordinary synergy of light weight, high stiffness, high strength and high toughness even though these properties are generally mutually exclusive.[2] As for artificial structural materials, similar structures have also been designed in order to overcome the ultrahigh-strength-but-ultra-low-ductility dilemma in ultrafine/nano-grained metals.[3,4] For example, a grain size gradient structure, in which the grain size varied by three orders along the sample thickness, has been introduced in the coarse-grained sample surface to generate strong synergetic hardening and strengthening.[5–10] Another example is a hierarchically nanotwinned (HNT) structure, in which secondary or even tertiary twin lamellae in a nanoscale were produced in the primary twin lamellae during plastic deformation.[11–13] The HNT structure exhibited exceptional properties and novel deformation modes as compared with the individually nanotwinned (NT) metals [14,15]; for

example, a combination of hierarchical and gradient NT structure offered a twinning-induced plasticity steel sample of doubled yield strength at no reduction in tensile ductility.[16] Therefore, manufacturing of HNT structures is a new approach to produce advanced materials with both high strength and high ductility.

To-date, researchers have performed a few theoretical and molecular dynamics (MD) simulations to reveal the deformation mechanism and mechanical behavior in HNT metals. Zhu et al. [17,18] have shown in their theoretical analysis that the existence of the HNT structure could give rise to an additional enhancement of strength. Moreover, two softening stages were observed in a MD simulation for a copper sample due to two transitions of deformation mechanisms with the decrease in primary twin spacing.[19] It is also interesting to note that detwinning of a secondary twin lamellae in a copper sample was observed in the MD simulations carried out by Yuan et al. [20] as the secondary twin spacing was reduced below a critical value. A rigorous investigation performed by Yuan et al. [21] clearly demonstrated that the presence of secondary twins could significantly

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toughen the HNT Cu sample because of crack blunting arising from detwinning of secondary twin lamellae, as well as dislocation emission from the primary and secondary twin boundaries as the secondary twin spacing was small. Inspired by the above findings and in view of the prevalence of detwinning or twin boundary (TB) migration in NT [22–25] and HNT [19–21] metals, an attempt will be made in this letter to develop a theoretical model, by extending the model of Ovid'ko and Sheinerman,[26,27] to investigate the effect of the detwinning behavior on crack blunting in HNT metals. The fracture toughness of the HNT metal with detwinning of the secondary twin lamellae dominating is also discussed.

Consider a deformed elastically isotropic HNT specimen with a long flat mode I crack embedded, which is subjected to an applied tensile stress σ , as shown in Figure 1(a). The HNT structure contains both primary and secondary twin lamellae of high density, whose thicknesses are denoted as λ_1 and λ_2 , respectively, as shown in Figure 1(b). For simplicity, a two-dimensional cracked ultrafine/nano-grained structure with the crack tip located at the primary TB segment BF (Figure 1(b)) is analyzed. The crack is assumed to nucleate and propagate along the primary TB segment BF, as observed in MD simulations,[21,28] due to the low TB energy. The applied load and the stresses induced at the crack tip are assumed to be sufficiently high (the shear stress is estimated to be around 700 MPa according to existing experimental measurements [24,25]) to initiate detwinning of the secondary twin lamellae ABFE (Figure 1(c) and (d)), which is accompanied by the migration of the secondary TB AB, as observed in the MD simulations.[21] The detwinning process or the TB migration process, which is different from the mechanism of grain boundary (GB) migration,[29–32] could be achieved by the travelling of the Shockley partials on the TBs, as validated by various experiments [23–25] and MD simulations.[19–22]

In the present HNT structure, when the first Shockley partial \mathbf{b}_p is emitted from the primary TB segment BF, it glides on the secondary TB AB and finally stops at another primary TB segment AE, while its trailing counterpart $-\mathbf{b}_p$ stays at the primary TB segment BF as observed in MD simulations [19,21] and experiments [23–25] and, hence, the secondary TB AB is moved to a new position A'B' by a distance δ (Figure 1(c)), where $\delta = a/\sqrt{3}$ is the distance between the neighboring slip planes and a is the crystal lattice parameter. The magnitude of Burgers vector of the partials is $b_p = a/\sqrt{6}$. The successive emissions and glides of \mathbf{b}_p ultimately result in two arrays of dislocations located in the primary TB segments BF and AE, which is accompanied by the migration of the secondary TB AB to a new position CD by a distance $m = n\delta/\sin\varphi$ (Figure 1(d)), where n is the number of partials emitted from the

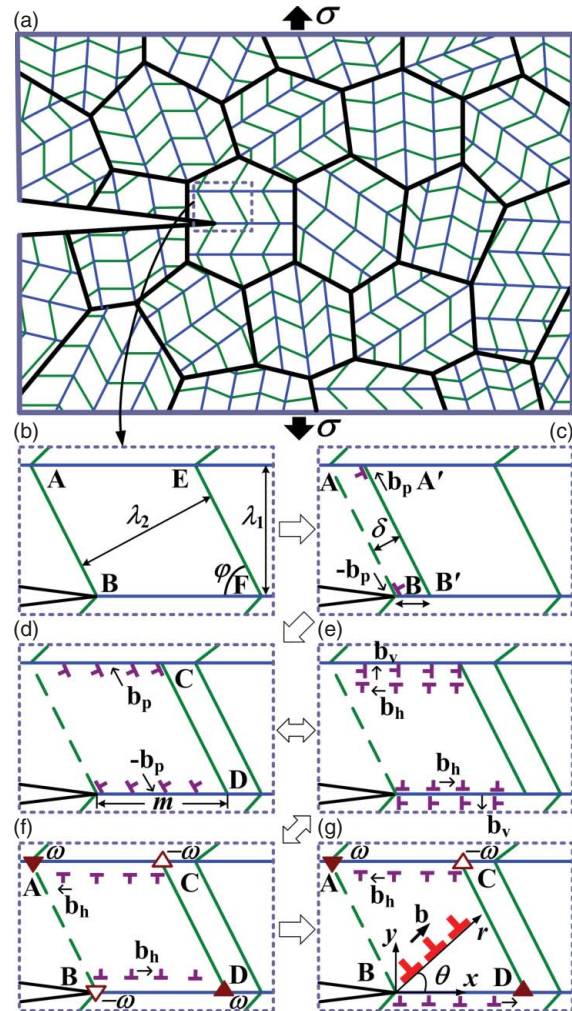


Figure 1. Lattice dislocation emission from a crack tip in a deformed hierarchically twinned (HNT) structure in which the detwinning behavior ((c) and (d)) is dominating: (a) general view; (b) magnified view of the HNT structure; (c) emission of a Shockley partial \mathbf{b}_p from the primary TB segment BF, which travels on the secondary TB AB with its trailing counterpart $-\mathbf{b}_p$ staying at the primary TB segment BF that leads to the normal migration of the secondary TB AB of distance δ ; (d) emission of successive partials from the primary TB segment BF produces two dislocation arrays along AC and BD lines, which are located at the primary TBs, and the subsequent motion of the secondary TB AB moves it to a new position CD by a distance m ; (e) presentation of the two dislocation arrays as the superposition of the dislocations with Burgers vectors \mathbf{b}_v and \mathbf{b}_h ; (f) equivalence of the stress fields induced by the two dislocation arrays with Burger's vector \mathbf{b}_v to those created by two dipoles of wedge disclinations AC and BD (denoted by triangles); (g) emission of dislocations with Burgers vector \mathbf{b} from the crack tip after the detwinning process.

primary TB segment BF. The two dislocation arrays could be presented as the superposition of the dislocations with Burgers vectors \mathbf{b}_v and \mathbf{b}_h , whose magnitudes are $b_v = b_p \sin\varphi$, $b_h = b_p \cos\varphi$, as shown in Figure 1(e). In accordance with the theory of defects in solids,[33] the

stress field induced by the two dislocation arrays with Burgers vector \mathbf{b}_v are equivalent to those created by two dipoles of wedge disclinations AC and BD with strength $\pm\omega$ ($\omega = 2\arctg(b_p \sin^2 \varphi / (2\delta))$) (denoted by triangles) (Figure 1(f)). In the limit of a semi-infinite crack, the disclination B and the dislocation at the crack tip become located at an external surface and thus disappear, in which case the disclination quadruple BDCA is transformed into three disclinations D, C and A, and the number of the dislocations at the primary TB segment BD is reduced from n to $n - 1$.

In order to consider the effect of detwinning of the secondary TB on crack blunting in a HNT specimen, we assume that the migration of the secondary TB AB is accompanied by emission of several edge dislocations with Burgers vector \mathbf{b} from the semi-infinite crack tip along the slip plane, as observed in MD simulations [21] and inclining at an angle θ with respect to the x -axis, as shown in Figure 1(g). The magnitude of Burgers vector of the emitted dislocations is $b=a/\sqrt{2}$. The total force acting on the first dislocation F_r^1 can be expressed as $F_r^1 = b\sigma_{r\theta}^e(r_1, \theta)$, where $\sigma_{r\theta}^e(r_1, \theta)$ is the effective stress and r_1 is the distance of the first dislocation from the crack tip. All dislocations have to overcome the crack tip attraction zone associated with the presence of the image stress induced by the crack in order to emit from the crack tip. According to Ovid'ko and Sheinerman,[26,27] if the first dislocation is repelled from the crack tip, it can be emitted whenever the distance from the dislocation to the crack tip exceeds the dislocation core radius r_c . Therefore, the emission criterion for the first dislocation is that the effective stress $\sigma_{r\theta}^e(r_1, \theta)$ at $r_1 = r_c$ should be larger than zero, that is,

$$\sigma_{r\theta}^{K_1}(r_1, \theta) + \sigma_{r\theta}^{\text{im}}(r_1, \theta) + \sum_{j=1}^3 \sigma_{r\theta}^{\omega}(r_1, \theta, r_j, \theta_j) + \sum_{j=1}^{2n-1} \sigma_{r\theta}^d(r_1, \theta, r_{dj}, \theta_{dj}) \Big|_{r_1=r_c} > 0, \quad (1)$$

where the stress $\sigma_{r\theta}^{K_1}(r_1, \theta)$ is induced by the applied tensile load near the crack tip; $\sigma_{r\theta}^{\text{im}}(r_1, \theta)$ depicts the image stress induced by the crack free surface; $\sigma_{r\theta}^{\omega}(r_1, \theta, r_j, \theta_j)$ is the stress induced by the j th disclination at point (r_j, θ_j) ($j = 1, 2, 3$ correspond to disclinations D, C and A, respectively); and $\sigma_{r\theta}^d(r_1, \theta, r_{dj}, \theta_{dj})$ represents the stress generated by the j th dislocation at point (r_{dj}, θ_{dj}) in the primary TB segments AE and BF. The first dislocation after emission is assumed to move along the slip plane and finally stops at the newly formed secondary TB CD as shown in Figure 1(g). Similarly, the $(N + 1)$ th dislocation ($N = 1, 2, \dots$) would be able to emit if there is a region within the interval $0 < r < \lambda_2$, where this dislocation is repelled from the crack tip, that is, the requirement for emission of the $(N + 1)$ th

($N = 1, 2, \dots$) dislocation is as follows:

$$\left. \begin{aligned} &\sigma_{r\theta}^{K_1}(r_{N+1}, \theta) + \sigma_{r\theta}^{\text{im}}(r_{N+1}, \theta) \\ &+ \sum_{j=1}^3 \sigma_{r\theta}^{\omega}(r_{N+1}, \theta, r_j, \theta_j) \\ &+ \sum_{j=1}^{2n-1} \sigma_{r\theta}^d(r_{N+1}, \theta, r_{dj}, \theta_{dj}) \\ &+ \sum_{j=1}^N \sigma_{r\theta}^{\text{de}}(r_{N+1}, \theta, r_{dej}, \theta_{dej}) \end{aligned} \right|_{r_{N+1}=r_c} > 0, \quad (2)$$

where $\sigma_{r\theta}^{\text{de}}(r_{N+1}, \theta, r_{dej}, \theta_{dej})$ is the stress exerted by the j th emitted dislocation at point (r_{dej}, θ_{dej}) on the newly emitted one. Here for simplicity, the emitted $N + 1$ dislocations are assumed to be uniformly distributed along the slip direction. This approximation should not affect the calculations significantly, as validated by our previous work.[34] The lengthy expressions of all the shear stresses that appear in Equations (1) and (2) are derived in the Supplementary Material (Section A).

In order to predict the maximum number of dislocations N_{max} emitted from the crack tip, the following procedure is adopted: (i) verify the possibility of emission of the first dislocation using Equation (1); (ii) if Equation (1) is satisfied, then employ Equation (2) to check the possibility of emission of the second dislocation; (iii) repeat step (ii) for the subsequent impending dislocations.

Moreover, in order to obtain an in-depth understanding of the toughening effect of detwinning of the secondary twin lamellae, the fracture toughness of the HNT Cu with or without dislocation emission from the crack tip was also calculated by incorporating the defect configuration formed due to the detwinning process and the dislocation emission process from the crack tip. By modifying the standard mode I brittle crack growth criterion,[35–38] which was established based on the balance between the driving force related to a decrease in elastic energy and the hampering force due to the creation of a new free surface during crack growth, an effective critical stress intensity factor K_{IC}^e is developed to account for the coupling effect of detwinning of the secondary twins and the slip of the dislocations emitted from the crack tip on crack growth. In this case, the propagation of crack is assumed to occur solely under the action of the tensile load perpendicular to the crack growth direction, while the presence of the disclinations and dislocations simply cause a change to the K_{IC}^e value. Therefore, the expression of K_{IC}^e for a plane strain state can be derived as what was done in our previous work [37]:

$$K_{\text{IC}}^e = \sqrt{(K_{\text{IC}}^{\sigma})^2 - (k_{\text{II}}^{\omega} + k_{\text{II}}^{\text{d}} + k_{\text{II}}^{\text{de}})^2} - (k_{\text{I}}^{\omega} + k_{\text{I}}^{\text{d}} + k_{\text{I}}^{\text{de}}), \quad (3)$$

where $K_{\text{IC}}^{\sigma} = \sqrt{4G\gamma_c/(1-\nu)}$ is the fracture toughness in a disclination-and-dislocation free case, in which brittle fracture occurs with the detwinning and dislocation emission process being completely suppressed; G and

ν are the shear modulus and Poisson's ratio, respectively; $\gamma_e = \gamma - \gamma_{TB}/2$ by assuming that the crack propagates along the TBs, as observed in MD simulations [28]; γ and γ_{TB} are the specific surface energy and TB energy, respectively. k_I^ω (k_{II}^ω), k_I^d (k_{II}^d) and k_I^{de} (k_{II}^{de}) are the stress intensity factors for the stress normal to crack line (or shear stresses) generated by the three disclinations, the dislocations located at the primary TB segments BD and AC, and the dislocations emitted from the crack tip, respectively (Figure 1(g)). These stress intensity factors are derived in the Supplementary Material (Section B).

The following parametric values of HNT Cu are adopted in the present calculation: $G = 46$ GPa, $\nu = 0.36$, $\gamma = 1.72$ J/m², [39] $\gamma_{TB} = 0.24$ J/m², $a = 0.362$ nm, $r_c \approx b$, $\theta = \pi/3$ and $\varphi = \pi/4$. The migration distance of the secondary TB AB is set as $m = \lambda_2/2$ to investigate the effect of the secondary twins on crack blunting.

The variation of the maximum number of dislocations N_{max} emitted from the crack tip with the secondary twin spacing λ_2 , for various primary twin thicknesses ($\lambda_1 = 10, 30$ and 50 nm), are presented in Figure 2, in which the results for a nanocrystalline (NC) Cu (i.e. N_{max} vs. grain size d) without HNT structure are also included for comparison. In this NC Cu sample, no detwinning or TB migration could occur due to the lack of HNT structure. The only factor that determines the capability to emit dislocations of a crack tip in NC Cu is the slipping space, that is, the grain size d . It can be seen that the values of N_{max} for a NC Cu are very small (≤ 2) even though the grain size is as large as 50 nm. Such low values of N_{max} lead to an ultra-low ductility as commonly observed in NC metals. In contrast, it is intriguing to find that the value of N_{max} in a HNT Cu could be increased significantly, and that the larger the

value of λ_1 is, the larger the N_{max} . The value of N_{max} could reach as high as 14 at $\lambda_2 = 14$ nm for the case of $\lambda_1 = 50$ nm, which is a great enhancement as compared with the case of NC Cu. This finding shows that slipping space is not the only factor that determines the capability of the crack tip to emit dislocations for HNT Cu; in fact, the formation of a proper defect configuration near the crack tip, for example, disclinations and dislocations formed due to the detwinning process of the secondary twin lamellae, as shown in Figure 1(g), plays a much more important role in enhancing the capability of the crack tip to emit dislocations than the slipping space. It is also important to note that the value of N_{max} for a HNT Cu first increases monotonously from zero to a maximum value and then decreases with decreasing secondary twin spacing λ_2 for all the primary twin thicknesses considered. Thus, one may infer that there exists a critical secondary twin spacing λ_{2c} , which increases from 9 to 14 nm as the primary twin spacing is increased from 10 to 50 nm. This is corresponding to an enhancement of N_{max} by a factor of 0.56 , that is, N_{max} is increased from 9 to 14 . By taking the case of $\lambda_1 = 30$ nm as an example, Figure 2 shows that N_{max} only exists when λ_2 is in the range of $(1, 34)$ nm, and the largest N_{max} (i.e. 11) occurs at $\lambda_2 = 10$ nm. These findings suggest that strong crack blunting by dislocation emission from the crack tip could be achieved at a small value of λ_2 , which could be optimized by tuning it to 10 nm in the HNT Cu, through detwinning of the secondary twin lamellae. The optimal λ_2 value of 10 nm is consistent with the existing experimental observation that detwinning usually occurred at twin thickness of several nanometers. [24,25] Thus, one may infer that HNT metals can be significantly toughened by detwinning the secondary twin lamellae at a nanoscale. This is in good agreement with the observations made by Yuan and Wu [21] in their recent MD simulations (refer to their Figure 8 that illustrated crack propagation along the primary TB). As a result, the great enhancement of N_{max} and the presence of an optimal N_{max} suggest that an effective crack blunting and toughening mechanism by hierarchical structure in ultrafine/nano-grained metals has been discovered theoretically.

The existence of optimal N_{max} in HNT metals, as shown in Figure 2, could be attributed to detwinning of the secondary twin lamellae since no such behavior was observed in the case without detwinning. As a matter of fact, upon examination of the effective stress created by detwinning, that is, the third and fourth terms in Equation (2), we find the trend of first-increase-and-then-decrease with decreasing λ_2 . This trend undoubtedly governs the variation of N_{max} with respect to λ_2 in the case where detwinning of the secondary twins is the dominating deformation mode. On the other hand, physically, when λ_2 is decreased to 20 – 30 nm, the dislocation

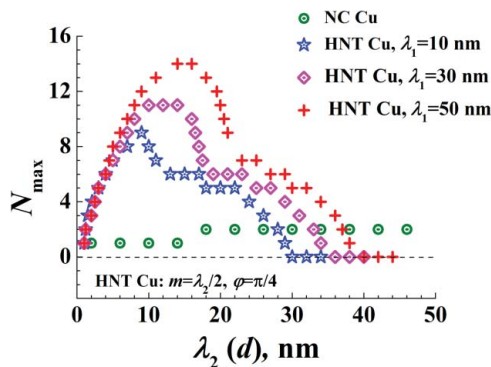


Figure 2. Variation of the maximum number of edge dislocations N_{max} emitted from the crack tip with respect to the secondary twin spacing λ_2 in a HNT Cu sample for three primary twin spacings, that is, $\lambda_1 = 10, 30$ and 50 nm. The results for a NC Cu (N_{max} vs. grain size d) are also included for comparison.

slips and pile-ups at GBs and TBs, which are usually prevalent in HNT metals with larger twin thickness, give way to detwinning of the primary and secondary twin lamellae.[20] Thus, in this case, the detwinning process enhances dislocation emissions from the crack tip and their pile-up at the secondary TBs, as shown in Figure 2. However, if λ_2 is reduced further, it becomes much more difficult for the emitted dislocations to pile up at the secondary TB in an extremely small twin thickness of size less than 5–10 nm due to space limitation even though detwinning could enhance emission of dislocations. Therefore, one may infer that the detwinning behavior of the secondary TBs plays an optimal role at a critical λ_2 of around 10–15 nm in blunting crack in HNT metals.

Figure 3 presents the variation of the effective stress intensity factor K_{IC}^e given by Equation (3) for the case of detwinning (DT only) and the combination of detwinning and the profuse dislocations emitted from the crack tip (DT + Disl. emiss.) with respect to the secondary twin spacing λ_2 of HNT Cu for three cases of λ_1 , that is, $\lambda_1 = 10, 30$ and 50 nm. An improved toughening behavior is achieved if $K_{IC}^e/K_{IC}^\sigma \geq 1$. It can be seen from Figure 2 that all curves for DT + Disl. emiss. cases exhibit a trend of first-increase-and-then-decrease with the decrease of λ_2 , and the maximum K_{IC}^e/K_{IC}^σ occurs at 2.5, 3 and 5 nm, respectively, for the three λ_1 values considered. This shows that the optimal toughening effect of the HNT structure can be achieved at $\lambda_2 \leq 5$ nm for HNT Cu with $\lambda_1 \leq 50$ nm. The critical λ_2 for optimal fracture toughness differs from that for optimal capability to emit dislocations from a crack tip because an optimal crack blunting capability does not necessarily lead to an optimal fracture toughness. This value is in excellent agreement with the

existing experimental and MD observations that twin lamellae with thickness smaller than 5 nm were usually detwinned.[19–21,23–25] It is also important to note that the thicker the primary twin lamella is, the higher is the maximum K_{IC}^e/K_{IC}^σ . Specifically, the maximum value of K_{IC}^e/K_{IC}^σ increases from 3.73 to 6.97, that is, an 87% enhancement, as λ_1 is increasing from 10 to 50 nm. Moreover, Figure 3 also illustrates that detwinning itself could significantly enhance the fracture toughness. The subsequent dislocations emitted from the crack tip due to the detwinning process could further toughen the materials. The maximum K_{IC}^e/K_{IC}^σ can be increased by around 40% because of these emitted dislocations for the cases of $\lambda_1 = 30$ and 50 nm. As a result, the significant enhancement of the fracture toughness due to the coupling effect of detwinning and emission of dislocations from a crack tip indicates that the HNT structure with a comparably larger primary twin thickness is very effective in toughening ultrafine/nano-grained metals.

The existence of optimal effective fracture toughness in HNT metals can be explained as follows. On the one hand, our further calculations have shown that the first-increase-and-then-decrease trend results from the variation of the second term in the square root of Equation (3), that is, contribution from the detwinning and the dislocation emission. On the other hand, physically, it is the competition between the detwinning process and the limited space that produces an optimal fracture toughness. As the twin thickness is decreased below 10–20 nm, the detwinning process begins to play an important role in enhancing the fracture toughness of HNT metals. However, as the twin size is reduced below 2–5 nm, the role of the detwinning process is suppressed in an extremely small space due to the mutual interactions of disclinations and dislocations. Therefore, it is conceivable that the detwinning behavior of the secondary TBs plays an optimal role at a critical λ_2 of around 5 nm in toughening HNT metals.

In summary, a theoretical model has been successfully developed to investigate the effect of detwinning of the secondary twin lamellae on crack blunting in HNT metals. The results obtained show that the detwinning behavior can greatly enhance the maximum number of dislocations emitted from a semi-infinite crack tip, which facilitates strong crack blunting and thus improves the ductility of HNT metals. Moreover, the detwinning process can significantly enhance the effective stress intensity factor and its toughening effect could be optimized as the secondary twin spacing λ_2 is reduced to 2–5 nm, which is in excellent agreement with the experimental and MD observations.[19–21,23–25] In conclusion, the proposed model reveals a new toughening mechanism by the hierarchical structure in ultrafine/nano-grained metals and could help to explain

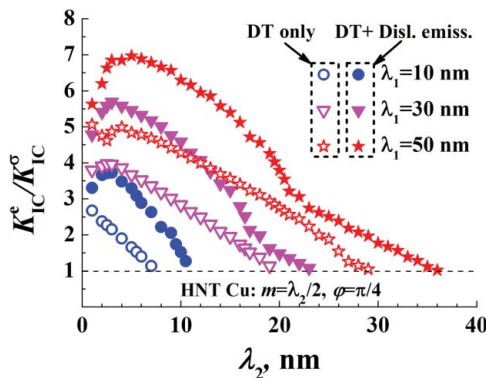


Figure 3. Variation of the normalized effective stress intensity factor K_{IC}^e/K_{IC}^σ for HNT Cu without and with dislocations emitted from the crack tip, as indicated by ‘DT only’ (detwinning) and ‘DT + Disl. emiss.’ (combination of detwinning and dislocations emitted from the crack tip), respectively, with respect to the secondary twin spacing λ_2 .

the exceptionally high ductility observed in the recently reported HNT metals.[11,16]

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Supplementary online material. A more detailed information on the proposed model is available at <http://dx.doi.org/10.1080/21663831.2015.1048905>.

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