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# FORMATION OF DEFORMATION TWINS THROUGH IDEAL NANOSHEAR EVENTS NEAR CRACK TIPS IN DEFORMED NANOCRYSTALLINE MATERIALS

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**Abstract.** Formation of deformation twins near crack tips in deformed nanocrystalline materials is theoretical described. Within the suggested model, deformation twins are generated and evolve through ideal nanoshear events carried by nanodisturbances and initiated by high local stresses in the vicinities of crack tips. The nanoscale twin formation releases in part local stresses near crack tips and thus hampers crack growth in pre-cracked nanocrystalline solids.

## 1. INTRODUCTION

Nanocrystalline and ultrafine-grained structures in solids are responsible for their specific mechanical, physical and chemical properties; see, e.g., [1-15]. For instance, plastic deformation processes and their micromechanisms in nanocrystalline metals and ceramics in many aspects are different from those in their conventional coarse-grained counterparts; see, e.g., book [1] and reviews [2-5]. This difference is due to both very small sizes of grains and large amounts of grain boundaries (GBs) in nanocrystalline materials, in contrast to large grains and negligibly low volume fractions occupied by GBs in coarse-grained polycrystals. In particular, deformation twinning represents a typical deformation mode in nanocrystalline materials where the formation of nanoscale twins has its specific features; for a review, see [16]. In doing so, formation of deformation twins is typically enhanced in nanocrystalline materials (compared to coarse-grained polycrystals), and such twins are often generated at GBs [16]. One of important factors that favor enhanced deformation twinning in nanocrystalline materials represents operation of very high stresses in such materials during plastic deformation. In this context, it is interesting to understand and describe formation of nanoscale deformation twins in areas near crack tips, where high local stresses operate in nanocrystalline materials. Recently, formation of nanoscale twins in crack-free solids at high stresses has been described as a process being realized through either consequent or simultaneously occurring ideal nanoshear events [17,18] and serving as an effective alternative to conventional twin formation mechanism [16,19-23] in nanocrystalline materials, the namely twin formation related to emission of partial dislocations from GBs. The main aims of this paper are to suggest a theoretical model describing formation of deformation twins through ideal nanoshear events near crack tips in nanocrystalline materials and to estimate its effect on fracture toughness of such materials.

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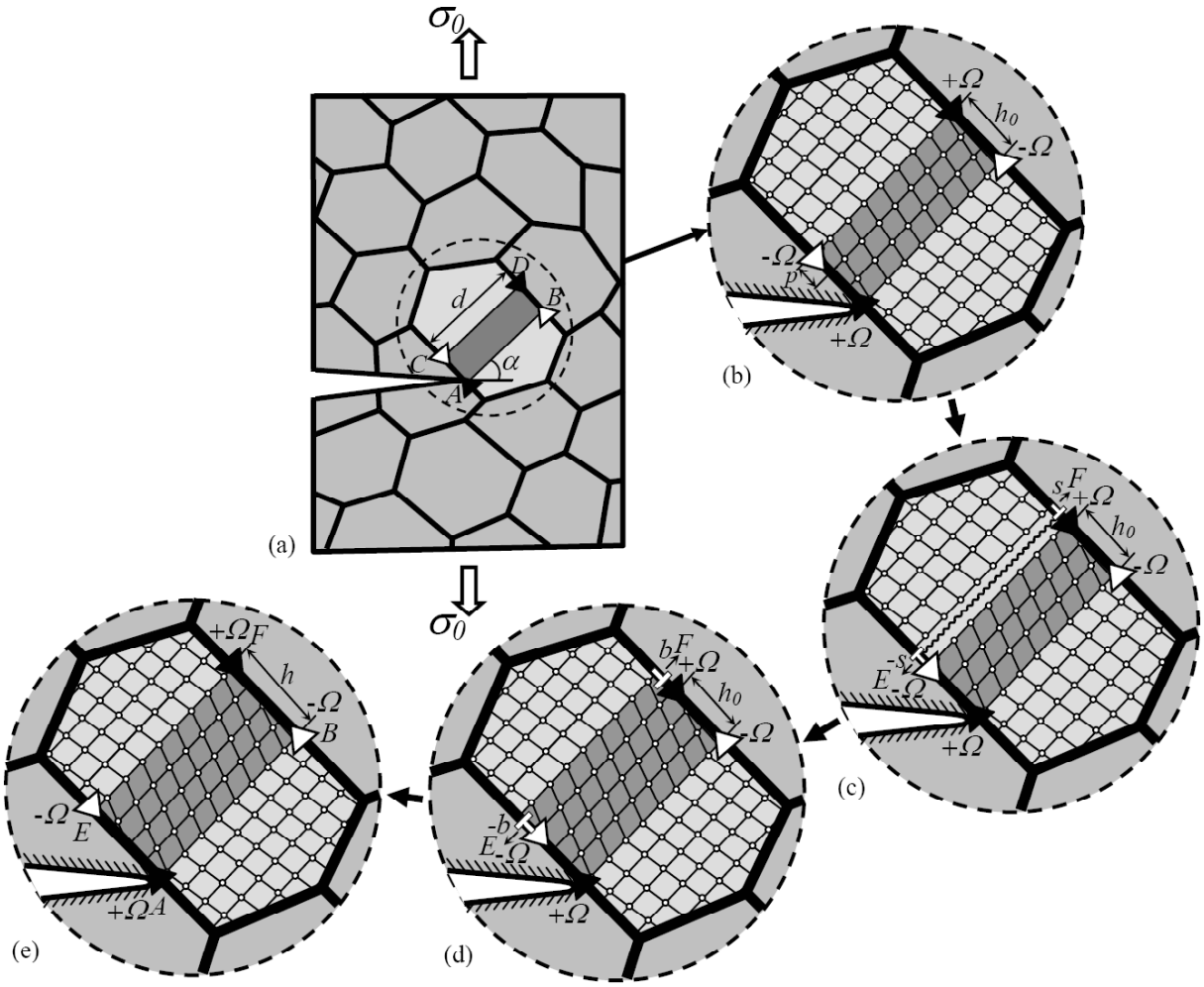


**Fig. 1.** Nanotwin growth in a deformed nanocrystalline specimen containing a pre-existent crack (a two-dimensional model). (a) General view. A deformed nanocrystalline specimen contains both a crack and a rectangular nanotwin *ABCD*. The nanotwin as a stress source represents a quadrupole of wedge disclinations located at its vortices. (b) The atomic structure of the grain contains the nanotwin *ABCD* in its initial state (schematically). (c) A dipole *EF* of partial non-crystallographic dislocations with the growing Burgers vector magnitude *s* is generated in the crystal plane adjacent to the twin boundary CD. (d) The Burgers vector magnitude *s* of the dipole dislocation gradually increases and reaches the magnitude *b* of the Burgers vector of a Shockley partial. (e) As a result, the length of the nanotwin *ABCD* increases, and the nanotwin *ABCD* transforms into the nanotwin *ABEF*.

## 2. FORMATION AND GROWTH OF A NANOTWIN NEAR A CRACK TIP IN A NANOCRYSTALLINE SOLID. MODEL

Let us consider a nanocrystalline solid consisting of nanoscale grains divided by GBs. Let the solid be under a remote tensile load s and contain a mode I crack whose tip approaches a GB. A two-dimensional section of the solid is schematically presented in Fig. 1a. For the aims of this study, it is sufficient to use a two-dimensional picture that takes into account all key aspects of the twin formation process under our consideration.

Within our model, the mode I crack of length *l* concentrates the external stress near its tip, and the resulting local stress induces generation of a deformation twin *ABCD* (Figs. 1a and 1b). Following the approach [18], the deformation twin near the crack tip is generated and evolves through the events of ideal nanoscale shear consequently occurring on parallel glide planes, as it is schematically shown in Fig. 1. In terms of dislocations, the twin formation process (Fig. 1) is represented as consequent generation of *n* dislocation dipoles on parallel glide planes. In doing so, generation of each dislocation dipole is realized through both growth of the magnitude *s* of the Burgers vectors of its dislocations

from 0 to $b$ (with $b$ being the magnitude of the Shockley partial) and corresponding evolution of generalized stacking faults located between immobile dislocations composing the dipole. (Such dipoles of dislocations with gradually growing Burgers vector magnitudes are called nanodisturbances [24,25]. They or their 3-dimensional analogs having loop geometry were experimentally observed in deformed Gum Metals [26], micropillars [27] and nanowires [28]; see also theoretical papers [18, 29-31].) The nanoscale twin *ABCD* (Fig. 1a) resulted from $n$ ideal nanoshear events creates internal stresses in the specimen. Following the approach [18], the twin *ABCD* (Fig. 1a) as a stress source can be effectively represented as a quadrupole of wedge disclinations characterized by strengths $\pm\Omega$ (hereinafter called $\pm\Omega$-disclinations) (Fig. 1b). In doing so, according to the theory of disclinations [32,33], the disclination strength magnitude $\Omega$ is in the following relationship with $b$ and the distance $p$ between neighboring dislocation dipoles: $\Omega = 2\arctan(b/2p)$. The nanoscale twin *ABCD* is supposed to have a rectangular shape with the sizes $d$ and $h_0$ (Figs. 1a and 1b) called also the disclination quadrupole arms. The distance $p$ between the neighboring dipoles of $\pm s$-dislocations is equal to the distance between the {111} crystal planes and related to the crystal lattice parameter $a$ by the equality $p = a/\sqrt{3}$. Within our model, the examined Shockley partials are edge dislocations with the Burgers vectors of the $(a/6)\langle 11\bar{2}\rangle$ type. The magnitude $b$ of such Burgers vectors is equal to $a/\sqrt{6}$.

Let the nanotwin *ABCD* consisting of $n$ dipoles of Shockley partials grow through the formation of $(n+1)$-st dipole *EF* of Shockley partials adjacent to the pre-existent nanotwin near a crack tip (Fig. 1c). As it has been discussed above, we assume that the dipole *EF* of Shockley partials forms via the growth of the magnitude $s$ of the Burgers vectors of its dislocations from 0 to $b$ and corresponding evolution of generalized stacking faults located between these immobile dislocations composing the dipole (Figs. 1c and 1d). As a result, the length $h_0$ of the nanotwin *ABCD* increases by $p$ (the distance between the {111} crystal planes). In other words, the new nanotwin *ABEF* forms which has the length $h = h_0 + p$ (Fig. 1e). Within our model, the above process of the nanotwin growth repeats until its further growth stops to be energetically favored. In order to estimate the conditions for energetically favorable nanotwin growth near a crack tip, in the following section, we will calculate the energy characteristics of the nanotwin growth (Fig. 1).

## 3. ENERGY CHARACTERISTICS OF NANOTWIN GROWTH NEAR A CRACK TIP IN A NANOCRYSTALLINE SOLID

Let us calculate the energy change due to the generation of a dipole *EF* of the partial $\pm s$-dislocations (Figs. 1c-1e) in a nanocrystalline solid containing a crack and a pre-existent nanotwin *ABCD*. The energy change $\Delta W$ (per dislocation unit length) can be presented as

$$\Delta W = E^{s} + E^{s-q} + E^{s-\sigma} + E_{\gamma}, \tag{1}$$

where $E^{s}$ denotes the self-energy of the dipole of $\pm s$-dislocations, $E^{s-q}$ designates the energy of the interaction between the stress fields of the dipole *EF* of the $\pm s$-dislocations and the quadrupole *ABCD* of wedge disclinations with the strengths $\pm\Omega$, $E^{s-\sigma}$ specifies the energy of the interaction of the dipole *EF* of the $\pm s$-dislocations with the stress field $\sigma_{ij}^{C}$ created by the applied load $\sigma_0$ in the solid with a crack, and $E_{\gamma}$ is the energy of the generalized stacking fault that joins the dipole dislocations.

In a first approximation, we neglect the effect of the crack on the energy $E^{s}$. Then the energy $E^{s}$ is calculated as the energy of a dislocation dipole in an isotropic solid [34]:

$$E^{s} = Ds^{2}\left(\ln\frac{d}{r_c} + 1\right), \tag{2}$$

where $D = G/[2\pi(1-\nu)]$, $G$ is the shear modulus, $\nu$ is Poisson's ratio, and $r_c \approx s$ is the dislocation core cutoff radius.

The energy $E^{s-q}$ of the elastic interaction between the disclination quadrupole and the dipole of $\pm s$-dislocations can be calculated as the work spent to the generation of the dislocation dipole in the stress field of the disclination quadrupole [33,34]. For the calculation of the energy $E^{s-q}$ we will also neglect the presence of the crack. Then the final expression for the energy $E^{s-q}$ follows as:

$$E^{s-q} = D\Omega b\left(h\ln\frac{d^2+h^2}{h^2} - p\ln\frac{d^2+p^2}{p^2}\right). \tag{3}$$

The energy $E^{s-q}$ can be written as [32]:

$$E^{s-\sigma} = -b\int_0^d \sigma_{xy}^{c}\,\mathrm{d}x, \tag{4}$$

where $\sigma_{xy}^{C}$ is the component of the stress field $\sigma_{ij}^{C}$ (see, e.g., [35]) created by the applied tensile load $\sigma_0$ in the solid with a flat crack of length $l$.

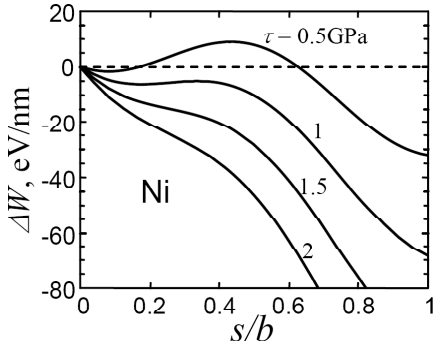


**Fig. 2.** Dependences of the energy change $\Delta W$ related to the generation of the dipole of non-crystallographic dislocations (in the plane adjacent to the nanotwin) on the normalized magnitude $s/b$ of the dipole dislocation Burgers vector, for various values of the applied shear stress $\tau$.

The energy $E_\gamma$ of the generalized stacking fault that joins the opposite dislocations with the Burgers vectors **±s** and is adjacent to $n$ stacking faults that compose the nanotwin *ABCD* is given [36,37] by

$$E_\gamma = \gamma_{n+1}(s)d, \tag{5}$$

where

$$\gamma_n(s) = \left(\gamma_{ut} - 2\gamma_{tsf}\right)\sin^2\left(\pi s/b\right), \quad n \geq 3, \tag{6}$$

$$\gamma_1(s) = \begin{cases} \gamma_{us}\sin^2\left(\pi s/b\right), & 0 \leq s/b \leq 1/2, \\ \gamma_{isf} + \left(\gamma_{us} - \gamma_{isf}\right)\sin^2\left(\pi s/b\right), & \\ \qquad 1/2 < s/b \leq 1, & \end{cases} \tag{7}$$

$$\gamma_2(s) = \begin{cases} \left(\gamma_{ut} - \gamma_{isf}\right)\sin^2\left(\pi s/b\right), & \\ \qquad 0 \leq s/b \leq 1/2, & \\ \left(\gamma_{ut} - \gamma_{tsf}\right)\sin^2\left(\pi s/b\right), & \\ \qquad 1/2 < s/b \leq 1, & \end{cases} \tag{8}$$

with $\gamma_{ut}$, $\gamma_{tsf}$, $\gamma_{us}$, and $\gamma_{isf}$ being the material constants.

Now the characteristic energy change $\Delta W$ is given by formulae (1) to (8). Let is calculate the dependence $\Delta W(s/b)$ in the exemplary case of nanocrystalline Ni. For Ni, we use the following parameter values: $G$ = 73 GPa, $\nu$ = 0.34, $a$ = 352 nm [38], $\gamma_{ut}$ = 0.324 J/m$^2$, $\gamma_{tsf}$ = 0.055 J/m$^2$, $\gamma_{us}$=0.273 J/m$^2$, and $\gamma_{isf}$ = 0.110 J/m$^2$ [36]. The dependences $\Delta W(s/b)$ for nanocrystalline Ni are plotted in Fig. 2, for $d$ = 20 nm, $l$ = 100 nm, $n$ = 10, $\alpha$ = 70°, and various values of the applied shear stress $\tau$. (The applied shear stress $\tau$ is defined here as the shear stress that would be created by the applied tensile load $\sigma_0$ in the crack plane in the absence of this crack, that is, $\tau = \sigma_0 \sin\alpha\cos\alpha$.) As it follows from Fig. 2, at $\tau$ = 0.5 GPa or 1 GPa, the energy change $\Delta W$ is not a monotonously decreasing function of $s$ being in the range $0 < s/b < 1$. That is, at these values of the shear stress $\tau$, the formation of a new dipole of the Shockley partials (with $s/b = 1$) requires surmounting an energy barrier. In contrast, at larger values of $\tau$ (1.5 GPa or 2 GPa), $\Delta W$ monotonously decreases with an increase in $s/b$ being in the range $0< s/b <1$. This implies that in the discussed situation, the formation of a new dipole of Shockley partials (necessary for the growth of the nanotwin *ABCD*) does not require overcoming an energy barrier. The analysis demonstrates that for the parameter values used to plot the curves in Fig. 2, the non-barrier nanotwin growth is realized at shear stresses $\tau$ exceeding 1.2 GPa.

## 4. EFFECT OF DEFORMATION NANOTWINNING ON FRACTURE TOUGHNESS OF NANOCRYSTALLINE SOLIDS

Let us examine the effect of nanotwinning on fracture toughness characteristics of nanocrystalline solids. To do so, consider an individual nanotwin *ABEF* (see Fig. 1) formed near the tip of a flat mode I crack in a nanocrystalline solid. The formation of the nanotwin is accompanied by the formation of the quadrupole of ±Ω-disclinations whose stress field influences crack growth. In order to examine the effect of the disclination quadrupole on crack propagation, we use the energy criterion of crack growth. In the considered case of the plane strain state, this criterion has the following form [39]:

$$\frac{1-\nu}{2\mu}\left(K_{\mathrm{I}}^2 + K_{\mathrm{II}}^2\right) = 2\gamma_e, \tag{10}$$

where $K_{\mathrm{I}}$ and $K_{\mathrm{II}}$ are the stress intensity factors, $\gamma_e = \gamma$ (where $\gamma$ is the specific surface energy) for an intragrain crack, and $\gamma_e = \gamma - \gamma_b/2$ (where $\gamma_b$ is the specific grain boundary energy) for a grain boundary crack, that is, a crack growing along a GB. In the considered situation where the crack propagates in the direction normal to the direction of the applied tensile load $\sigma_0$, the stress intensity $K_{\mathrm{I}}$ and $K_{\mathrm{II}}$ can be presented as

$$K_{\mathrm{I}} = K_{\mathrm{I}}^{\sigma} + k_{\mathrm{I}}^{\sigma}, \quad K_{\mathrm{II}} = k_{\mathrm{II}}^{q}, \tag{11}$$

where $K_{\mathrm{I}}^{\sigma}$ is the stress intensity factor associated with the applied load $\sigma_0$, while $k_{\mathrm{I}}^{q}$ and $k_{\mathrm{II}}^{q}$ are the

stress intensity factors associated with the stress field of the disclination quadrupole (Fig. 1e).

The local plastic deformation related to the formation of the nanotwin influences crack advance. This influence can be accounted for through the introduction of the critical stress intensity factor $K_{IC}$. In this case, the crack is considered as that propagating under the action of the tensile load perpendicular to the crack growth direction, while the presence of the disclination quadrupole simply changes the value of $K_{IC}$ compared to the case of brittle crack propagation. As a result, the critical condition for the crack growth can be represented as [40]:

$$K_{I}^{\sigma} = K_{IC}. \tag{12}$$

Substitution of (11) to (10) and account for formula (12) now yield [41]

$$K_{IC} = \sqrt{\left(K_{IC}^{\sigma}\right)^2 - \left(k_{IIC}^{q}\right)^2} - k_{IC}^{q}, \tag{13}$$

where

$$k_{IC}^{q} = k_{I}^{q}\Big|_{K_{I}^{\sigma}=K_{IC}},\ k_{IIC}^{q} = k_{II}^{q}\Big|_{K_{I}^{\sigma}=K_{IC}},\ \text{and}$$

$$K_{IC}^{\sigma} = \sqrt{4G\gamma_e/(1-\nu)}$$

is the fracture toughness in the case of brittle fracture, that is, in the situation where the disclination quadrupole is absent. In order to analyze the effect of the formation of the nanotwin *ABEF* on crack growth, one has to compare the quantities $K_{IC}$ and $K_{IC}^{\sigma}$. The relation $K_{IC} > K_{IC}^{\sigma}$ implies that the nanotwin formation leads to an increase in the fracture toughness of the nanocrystalline solid. If $K_{IC} < K_{IC}^{\sigma}$, the fracture toughness of the nanocrystalline solid decreases due to the nanotwin formation.

Let us calculate $K_{IC}$ in the case shown in Fig. 1e, where a disclination quadrupole is generated near the crack tip. We assume that the quadrupole arms *h* and *d* are small compared to the crack length *l* (*h*,*d*<<*l*). This allows one to consider this crack as a semi-infinite one in the calculation of the stress intensity factors $k_{I}^{q}$ and $k_{II}^{q}$. In the examined case of a semi-infinite crack, the disclination located at the crack tip (at the point A) turns out to be at the outer surface of the solid and disappears.As a corollary, the disclination configuration consists of three individual disclinations, but does not represent a disclination quadrupole. For this disclination configuration (Fig. 1e), the stress intensity factors $k_{I}^{q}$ and $k_{II}^{q}$ are calculated as follows [41]:

$$\begin{aligned}
&k_{I}^{q} = G\omega\sqrt{d}f_1(\alpha,t)/\left(2\sqrt{2\pi}(1-\nu)\right),\\
&k_{II}^{q} = G\omega\sqrt{d}f_2(\alpha,t)/\left(2\sqrt{2\pi}(1-\nu)\right),\\
&f_1(\alpha,t) = \sum_{k=1}^{3}(-1)^k\sqrt{\tilde{r}_k}\left[3\cos\left(\theta_k/2\right) + \cos\left(3\theta_k/2\right)\right],\\
&f_2(\alpha,t) = \sum_{k=1}^{3}(-1)^k\sqrt{\tilde{r}_k}\left[\sin\left(\theta_k/2\right) + \sin\left(3\theta_k/2\right)\right],
\end{aligned} \tag{14}$$

Where

$$\begin{aligned}
&t = h/d,\ \tilde{r}_2 = \sqrt{t^2+1},\ \tilde{r}_3 = t,\ \theta_1 = \alpha,\\
&\theta_2 = \alpha - \pi/2 + \operatorname{arccot} t + 2\pi\Xi\left(-\alpha - \pi/2 - \operatorname{arccot} t\right),\\
&\theta_3 = \alpha - \pi/2 + \operatorname{arccot} t + 2\pi\Xi\left(-\alpha - \pi/2\right),
\end{aligned}$$

$\Xi(x)$ is the Heaviside function equal to unity at $x \geq 0$ and zero otherwise.

Using formulae (13) and (14), let us calculate the ratio $K_{IC}/K_{IC}^{\sigma}$ as a function of the nanotwin dimensions *d* and *h*. The contour map of $K_{IC}/K_{IC}^{\sigma}$ in the coordinate space (*h*,*d*) is presented in Fig. 3 in the case of nanocrystalline Ni with $\gamma_e = \gamma = 1.725$ J/m$^2$ [38], $\alpha = 70°$ (see Fig. 1) and other parameter values specified above. The dashed arrow in Fig. 3 characterizes the variation in the nanotwin dimensions that corresponds to the highest possible value of $K_{IC}/K_{IC}^{\sigma}$. In other words, this arrow corresponds to the nanotwin dimensions at which the nanotwin maximizes the critical stress intensity factor $K_{IC}$ and thereby locally maximizes the fracture toughness of the nanocrystalline solid. Fig. 3 clearly demonstrates that the nanotwinning-related fracture toughness of the nanocrystalline solid increases when the nanotwin length *h* increases and/or grain size *d* decreases.

## 5. CONCLUDING REMARKS

Thus, formation and evolution of nanoscale deformation twins near crack tips in deformed nanocrystalline materials can effectively occur through ideal nanoshear events (Fig. 1). Our calculations have shown that the nanotwin growth through ideal nanoshear events carried by nanodisturbances is an energetically favorable process (initiated by high local stresses in the vicinities of crack tips) in nanocrystalline Ni in wide ranges of parameters characterizing its mechanical

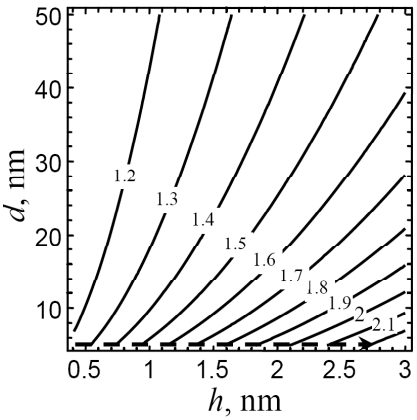


**Fig. 3.** Contour map of the normalized critical stress intensity factor $K_{IC}/K_{IC}^{\sigma}$ in the space ($h$,$d$) of nanotwin dimensions.

load and internal structures. In particular, the non-barrier nanotwin growth is realized in nanocrystalline Ni at local shear stresses t exceeding 1.2 GPa.

The nanoscale twin formation (Fig. 1) releases in part local stresses near crack tips and thus hampers crack growth in pre-cracked nanocrystalline solids. In doing so, as it has been demonstrated within our theoretical model, the nanotwinning-induced fracture toughness of a nanocrystalline solid increases when its grain size $d$ decreases and/or the nanotwin length $h$ increases (Fig. 3). Thus, the deformation nanotwinning through ideal nanoshear events near crack tips serves as an effective toughening micromechanism in nanocrystalline materials (where the conventional toughening micromechanism - lattice dislocation emission from crack tips [42,43] - is suppressed by GBs [44]). At the same time, its operation in conventional coarse-grained polycrystals is hardly effective, because the conventional toughening micromechanism [42,43] effectively comes into play at comparatively low level of local shear stresses near crack tips and thereby dominates over the nanotwinning.

## ACKNOWLEDGEMENTS

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