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# MATHEMATICAL MODELING OF GROWTH AND INTERACTION OF ELASTIC TWINS


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**Key words and phrases:** crack; elastic twin; modeling; twinning dislocation.



**Abstract:** Dislocation models of twins, represented by jogged positions of twinning dislocations at the boundaries, were examined. Uniform distribution of dislocations in an elastic twin, growing under the action of point load was calculated. Calculations of interaction of the contrary elastic twins were made. The results explain peculiarities of interaction of the contrary elastic twins observed during the experiment. Stresses which appeared in a zone surrounding the twin were determined. The manner of stress distribution allows explaining peculiarities of contrary twin interaction. In the experiment the formation of microcrack nucleation at distances up to 100 μm was observed. The microcrack nucleation can be caused by superposition field of tension stresses of interacting twins. Microcrack nucleation according to Fujita mechanism is considered to be more probable.


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## Introduction

The twins which come out of a crystal after unloading are named elastic twins. Such twins are formed under point load [1, 2]. In that case elastic stresses, in the field of which there is a growth of the twin, are not constant; they decrease as the distance from the zone of contact increases [3]

$$\tau = -\frac{2Px^2y}{\pi\left(x^2+y^2\right)^2}, \tag{1}$$

where $x$ and $y$ are the coordinates, $P$ is the force applied to the wedge and operating along $x$ direction.

In twinning boundaries the adjoining dislocations are located and move in the parallel planes shifted for distance $h$ [2]. Thus several dislocation models of twinning defects are possible [4]: single twinning border (**TB**), a twin with a disposition of dislocations which is symmetric regarding the plane of twinning (**ST**) and an asymmetric twin formed of boundaries with different number of dislocations (**AT**). In the present work mentioned models are analyzed using numerical method with reference to a problem of origin of destruction at mechanical twinning. Two schemes of microcrack nucleation – at the top of the stacked twin and at interaction of contrary twins are considered.

## Results and Discussion

The model of twinning boundaries is shown on Fig. 1. In generation of equations of dislocation balance in boundaries external stresses, stress of dislocation interaction and crystal resistance to a shift $\tau_S$ were considered. Equation of balance for the model on Fig. 1 can be written down as follows:

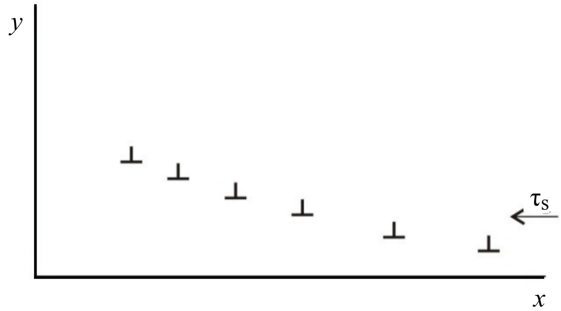


**Fig. 1. Dislocation model of a twin boundary**

$$A\sum_{j=1}^{n}\frac{(x_i-x_j)[(x_i-x_j)^2-(y_i-y_j)^2]}{[(x_i-x_j)^2+(y_i-y_j)^2]^2}+\frac{mA}{x_i}-\tau_S=0,\quad i=1,2,...,n, \qquad (2)$$

where $A=\dfrac{Gb}{2\pi(1-v)}$, $G$ is the module of shift, $v$ is Poisson's ratio, $b$ is Burgers vector of a single twinning dislocation, $x_i$ and $y_i$ are the coordinates of dislocations. If the twin is being broken at some obstacle, for example, at a twin of another system, then the equations of balance will be as follows

$$\frac{A}{x_i}+A\sum_{j=2}^{n}\frac{(x_i-x_j)[(x_i-x_j)^2-(y_i-y_j)^2]}{[(x_i-x_j)^2+(y_i-y_j)^2]^2}+\frac{mA}{x_i-L}=0,\quad i=2,3,...,n, \qquad (3)$$

where $L$ is the length of the twin.

For the twin with two boundaries the equations (2) are necessary to be supplemented with an item, mentioning the interaction of dislocations of different twin boundaries. In both equations an action of external loading is replaced by an elastic field of a superdislocation with the sum Burgers vector $mb$, located in the point $x = 0$. A basis of such replacement is the fact that the elastic fields created by point loading and stresses created by dislocation depend on the distance just as $1/x$. The loading $P$ can be calculated using the value $m$.

Some peculiarities of dislocation distribution for each model are illustrated by data on Fig. 2 (the twin is stopped). It is obvious, that most physically adequate model is the model AT. The model with a symmetric dislocation disposition is more likely to represents a special case. It is seen, that during the transformation of ST into AT the dislocations, situated symmetrically regarding the plane of twinning, are shifted to the opposite ends. Thus they are situated similarly to dislocations in TB with the number of dislocations equal to the sum of dislocations in the twin boundaries. At the analysis of freely growing twins which are hold back only by friction force, the model of a planar pile-up can provide acceptable accuracy. In the examination of the stacked twins the best description is provided by models AT, ST and TB accordingly.

In the view of crack nucleation in the stopped pile-up it is interesting to examine the dependence of distance between head dislocations $d$ on the applied stress $\tau$. It is shown, that for a constant external stress the latter can be presented by analytical expression for an arbitrary number of dislocations $n$. If we put $d$ from a condition of dislocation incorporation, we receive critical parameters of microcrack nucleation. Criterion of head dislocation incorporation at the forced approach is reaching the distance $d = 2.41h$ between them. Thermally activated crack nucleation occurs if head dislocations draw together at a distance, for which the energy of a pair kink formation in the second dislocation of a depth $(d - b)$ possesses a preset value (the order ~2 eV) [5].

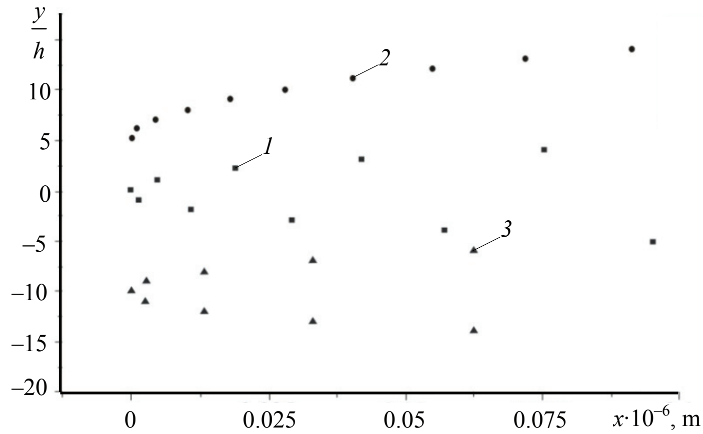


**Fig. 2. Disposition of dislocations at the top of defects:**
*1* – AT; *2* – TB; *3* – ST

In that case critical load is inversely proportional to number of dislocations in the twin. Conditions of microcrack nucleation in twinning defects appear to be less rigid, than in a stopped planar pile-up. Critical stresses of microcrack nucleation ($m$) for the elastic twin also decrease with the growth $n$. But the dependence of $m$ on $n$ becomes smaller. It is connected with the fact that in that case twin dislocations are situated in a decreasing field of elastic stresses.

The form of the free elastic twin (scaled) is shown on Fig 3. Here dislocation coordinates are marked on $x$ direction, and thickness of the twin (or number of dislocations in the boundary) – on $y$ direction. Comparing it with similar results for the stacked twin (Fig. 2), we can see that the top of the free twin is stretched in the direction of its movement and has the form of a pointed beak. Moreover, the form of the twin isn't changed as the friction stresses $\tau_S$ increase. The twin only decreases in its length inversely to the growth $\tau_S$.

For freely growing twins dislocation density is essentially smaller than it is required for head dislocation incorporation (~1/2.41$h$). Thus, if the growing twin hasn't met any obstacles, crack nucleation at its top according to the mechanism of dislocation incorporation is unlikely to happen. However, one point is necessary to be particularly mentioned. In fact, dislocations in a real twin are nonequivalent in the view of friction forces working on them. It is shown in [1] that the head dislocation is to be worked on by extra force of non-elastic origin, which is several times more than friction force for the rest of the twin dislocations.

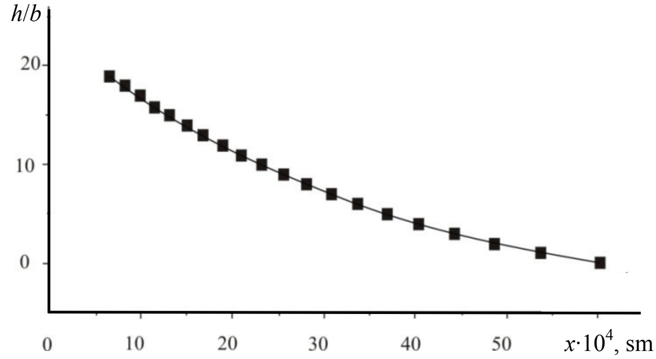


**Fig. 3. The form of twinning boundaries**

This circumstance makes a noticeable change in the dislocation distribution at the top of the twin (Fig. 4). Its form becomes obtuse and resembles the top of a stacked twin. This, in turn, leads to a sharp increase of dislocation density at its top. Unfortunately, there are no reliable estimates for the value of non-elastic forces. Therefore it is difficult to say whether their mentioning can lead to the crack nucleation at the top of a pile-up due to head dislocation incorporation.

Calculations of contrary twin interaction (Fig. 5) have been also made. In this part of the work the twins lying in parallel planes, which are situated at a distance $H$ apart, were examined. Twins were located in such a way that their tops were at a preset distance $\Delta l$ away from each other. Initial positions of dislocations were set by equilibrium coordinates of dislocations of a single twin. Then the twin was given an opportunity to relax to a new equilibrium position under the action of an elastic stresses field of another twin. The equilibrium form of the twins was found out depending on a level of the applied (value $m$) and geometrical parameters of $\Delta l$ and $H$ interaction. The equilibrium equations for the model in Fig. 5 are as follows:

$$\frac{mA}{x_i} + \sum_{j=1,\ j\neq i}^{n} \frac{A}{x_i - x_j} + \sum_{j=1,\ j\neq i}^{n} \frac{Ag_i(g_i^2 - H^2)}{(g_i^2 + H^2)^2} - \tau = 0, \quad i = 1, 2, ..., n, \tag{4}$$

$$g_i = \Delta l + 2L - x_i - x_j, \qquad \tau = \begin{cases} \tau_S, \, i \neq n, \\ \tau_f, \, i = n, \end{cases}$$

where a $\tau_f$ is the stress working on the head dislocation number $i = n$.

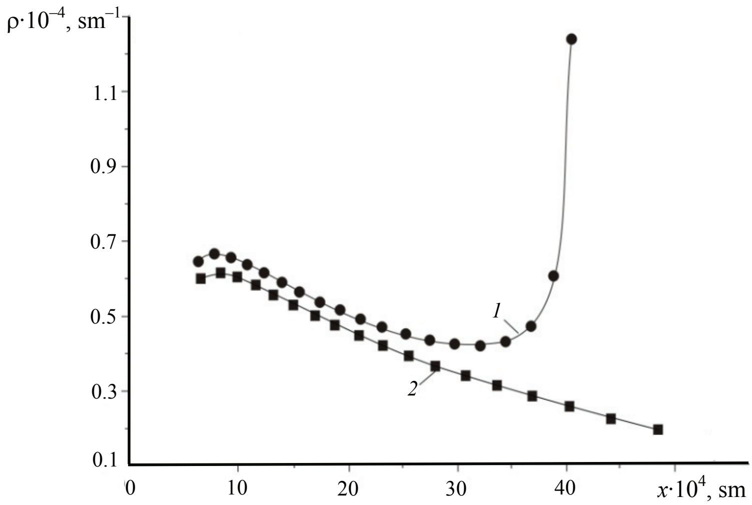


**Fig. 4. Density of twin dislocations**

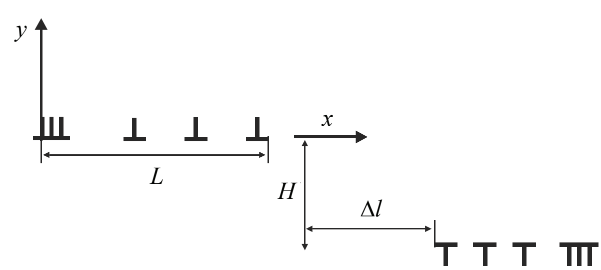


**Fig. 5. Dislocation model of contrary twin interaction**

Data in Fig. 6 show that the initial stage of twin interaction is the attraction. Calculations for $H/L = 10^{-4}$ were made, the initial length of twins was $3.5 \cdot 10^{-2}$ sm. Twins are attracted to each other almost to a complete closing of their tops, and then repulsion of head dislocations and reduction of the twin length is observed.

Peculiarity of twins is the fact that they consist of dislocations with identical Burgers vectors. Therefore at growth of the twin the field of long-range elastic stress in the twin surrounding field will be formed.

The shift stresses created by twins in planes of dislocation sliding of another twin (Fig. 7) were calculated. The manner of stress distribution enables to explain peculiarities of contrary twin interaction. They are, in particular, their attraction at initial closing and braking in process of twin layer (of the order 0.1…0.3 of their lengths). Besides, the effect of interaction is the stronger, the smaller the distance between planes of twin development is.

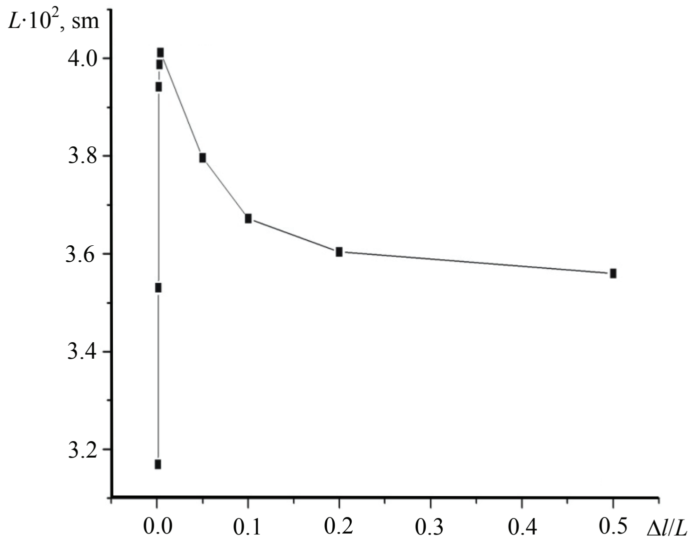


**Fig. 6. Dependence of the twin lengths on distance between the twin tops**

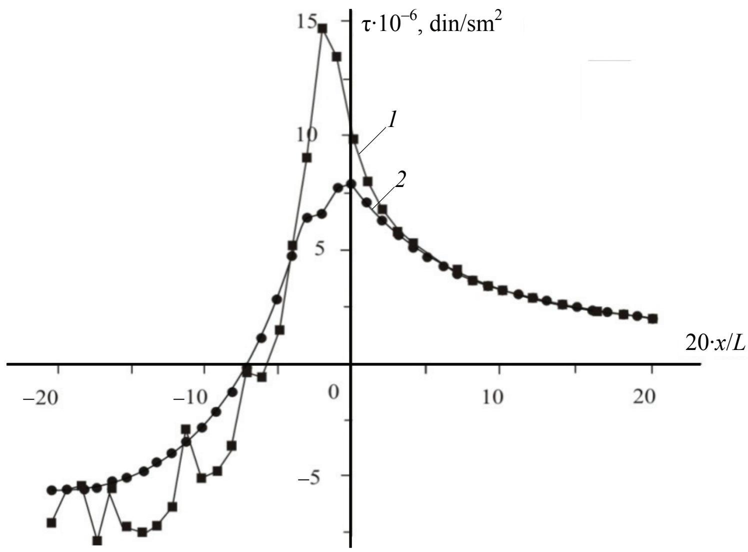


**Fig. 7. Shift stresses created by the twin in a plane parallel to a twinning plane:**
*1* – $H = 0.01L$; *2* – $H = 0.05L$

It is obvious that twin braking to a stop can be received only in case if their tops will be shifted on one interplane distance. And in this case the microcrack nucleation in the twin tops will occur as a result of the head dislocation incorporation. But the probability of such interaction is very little. In the experiment the formation of microcrack nucleation at distances $H$ up to 100 μm is observed. The microcrack nucleation can be caused by superposition field of tension stresses of interacting twins. Microcrack nucleation according to Fujita mechanism is considered to be more probable.

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## Математическое моделирование развития и взаимодействия упругих двойников


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**Ключевые слова и фразы:** двойникующая дислокация; моделирование; трещина; упругий двойник.



**Аннотация:** Рассмотрены дислокационные модели двойников, учитывающие ступенчатое расположение двойникующих дислокаций в границах. Рассчитано равновесное распределение дислокаций в упругом двойнике, растущем под действием сосредоточенной нагрузки. Выполнены расчеты взаимодействия встречных двойников. Результаты на качественном уровне хорошо объясняют особенности взаимодействия встречных двойников, наблюдаемые в эксперименте. Определены напряжения в области, окружающей двойник. Характер распределения напряжений позволяет объяснить особенности взаимодействия встречных двойников. В эксперименте наблюдается образование микротрещин на расстояниях до 100 мкм. Причина появления микротрещин – наложение полей растягивающих напряжений взаимодействующих двойников. Наиболее вероятным представляется вскрытие микротрещины по механизму Фудзиты.


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## Mathematische Modellierung der Entwicklung und der Wechselwirkung der elastischen Doppelgänger

**Zusammenfassung:** Es sind die Dislokationsmodelle der Doppelgänger, die die gestufte Anordnung der Doppelversetzungen in den Grenzen berücksichtigen, betrachtet. Es ist die Gleichgewichtsverteilung der Versetzungen im elastischen Doppelgänger berechnet, der unter dem Einfluß von der gesammelten Belastung wächst. Es sind die Berechnungen der Wechselwirkung der entgegenkommenden Doppelgänger erfüllt. Die Ergebnisse auf dem qualitativen Niveau erklären die Besonderheit der Wechselwirkung der entgegenkommenden Doppelgänger. Es sind die Anstrengungen auf dem die Doppelgänger umgebenden Gebiet bestimmt. Der Charakter der Verteilung der Anstrengungen lässt zu, die Besonderheit der Wechselwirkung der entgegenkommenden Doppelgänger zu erklären. Im Experiment wird die Bildung der Mikrorisse in den Entfernungen bis zu 100 mkm beobachtet. Der Grund des Erscheinens der Mikrorisse – das Auferlegen der Felder der ausbreitenden Anstrengungen der zusammenwirkenden Doppelgänger. Wahrscheinlichst wird das Öffnen des Mikrorisses nach dem Mechanismus von Fujita vorgestellt.

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## Modélage mathématique du développemt et de l'interaction des homologues élastiques

**Résumé:** Sont examinés les modèles de dislocation des homologues. Est calculée la répartition équilibre des dislocations dans les homologues élastiques. Sont exécutés les calculs de l'interaction des homologues contraires. Sont définies les tensions dans le domaine entourant les homologues. Le caractère de la répartition permet d'expliquer les particularités de l'interaction des homologues contraires. Dans l'expériment on observe l'apparition des microfissures à la distance jusqu'à 100 μm. La raison de l'apparition des microfissures est l'interposition des champs des tensions étendantes des homologues en interaction. La plus prévisible est l'ouverture de la microfissure à l'aide du mécanisme de Fujita.

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