# FRACTURE OF BRITTLE AND DUCTILE CRYSTALS FOR THE GENERALIZED STRESS STATE. STRENGTH AND DEFORMATION CRITERIA

V. M. Kornev

Lavrentyev Institute of Hydrodynamics, 630090, Novosibirsk, Russia

#### ABSRACT

Both growth and branching of sharp cracks in perfect crystals are studied (I and II fracture modes). Strength and deformation criteria of Neuber-Novozhilov type are proposed to describe sharp crack branching. A classification of materials by behavior types is given: brittle, quasi-brittle, quasi-ductile, and ductile behavior of materials under fracture. The classification is based on the angle characterizing the stress state on an imaginary plane. Curves of theoretical single crystal strength of the Coulomb-Mohr type for the generalized stress state on this theoretical plane are considered to be known. A possibility for multiple crack branching has been revealed that is related to the multiplicity of eigenvalues when buckling the system. It has been established that for perfect single crystals, the principle of the local symmetry is realized in the vicinity of the crack tip if the crystal symmetry axis coincides with the crack axis and the theoretical strength curve possesses the appropriate symmetry axis of a single crystal is inconsistent with the crack axis, the principle of the local symmetry fails.

Key words: Brittle fracture; Ductile fracture; Fracture criteria; Crack branching, Crack kinking; Principle of local symmetry

#### **1 INTRODUCTION**

Problems on steady-state growth of sharp cracks (or their branching) at some loading of a solid containing straight sharp crack is of certain interests. The complicated stress field is generated in the vicinity of a tip of a normal rupture crack. At certain conditions, blunting of sharp cracks can arise due to large shear stresses or deformations. For the time being, there is no defined answer to the question of whether is a sharp rupture crack stable in an perfect crystal due to shear stresses or shear deformations in the vicinity of a crack tip. How this stability is associated with ideal tensile or shear strength of a single crystal or limiting shear deformability of a crystal lattice?

Kelly et al. (1967) conceived the steady-state condition for a rupture crack in the form of the strength criterion (see Thomson, 1983; Knott, 1983). Rice and Thomson (1974) have supposed another steady-state condition for a rupture crack in the form of approximate relationship corresponding to the deformation criterion (see Thomson, 1983; Knott, 1983). We emphasize that the branching or blunting of cracks can occur, in general, in different places relative to the crack tip: for the strength criterion, crack branching occurs just ahead of the crack tip in material itself, and for deformation criterion, crack blunting occurs by shear at crack flanks.

### 2 STRESS FIELD AND DEFOMATION MODE IN TE VICINITY OF A CRACK TIP

Isotropic material containing an inner crack is considered at the microlevel as a material with the structure. An inner straight crack is modeled by the bilateral cut of length 2l. Let stresses  $\sigma_{\infty}$ ,  $\tau_{\infty}$  be specified at infinity for the crack of the first and second mode, respectively. We consider stability of crack growth to mean the problem of their branching. Assume that material considered has the symmetry of strength characteristics relative to the crack plane. In Fig. 1, the right tip of such a crack is shown with a solid line in the first quadrant and a dashed line shows the

tip of such a crack is shown with a solid line in the first quadrant and a dashed line shows the probable new location of the crack when it branches out, where  $\pm \theta^*$  are branching angles; points O and  $O_1$  correspond to previous and present locations of crack tips at the unit crack extension. At  $\theta^* = 0$ , a crack extends steadily in a straight line; at  $\pm \theta^* \neq 0$ , a crack branches out changing its direction, at  $\theta^* = \pm \pi/2$  the crack is blunted when it is opened. Unit advance of both brittle and ductile behavior of material under I fracture mode can be identified with angles  $\theta^* = 0$  and  $\theta^* = \pm \pi/2$ , respectively (see Kelly et al., 1967; Thomson, 1983; Knott, 1983; Rice and Thomson, 1974), but quasi-ductile ( $\theta^* = \pm \pi/2$ ) or quasi-brittle ( $\theta^* = \pm 0$ ) material behavior is possible, when  $\pm \theta^* \neq 0, \theta^* < \pi/2$ . We should emphasize that no restrictions are imposed in advance on behavior of the system except for the symmetry (as distinct from Kelly et al. (1967), Rice and Thomson (1974)). Therefore, generally speaking, such modes are possible when multiple branching occurs: for example,  $\theta_{21}^* \neq \theta_{22}^* \neq \theta_{23}^*$  (subscripts refer to numbers of the material structure and the loading type). Multiple branching is related to both the complexity of a stress fields in the vicinity of a crack tip and strength properties of isotopic material in the complicated stress state.



When crack branching is described, information about a stress field in the polar coordinates for the strength criterion needs to be determined, and for the deformation criterion, displacements of crack flanks in the rectangular coordinates Oxy in the vicinity of the crack tip should be known. The stress field and displacements of crack flanks in the vicinity of the right crack tip of normal rupture can be written in the form, see p. 15 - 17 from Savruk (1988),

$$\sigma_{\theta}(r,\theta) = (K_{\rm I}/\sqrt{2\pi r})\cos^{3}(\theta/2) - (K_{\rm II}/\sqrt{2\pi r})3\sin(\theta/2)\cos^{2}(\theta/2) + O(r^{0}),$$
  

$$\tau_{r\theta}(r,\theta) = (K_{\rm I}/\sqrt{2\pi r})\sin(\theta/2)\cos^{2}(\theta/2) + (K_{\rm II}/\sqrt{2\pi r})[1 - 3\sin^{2}(\theta/2)]\cos(\theta/2) + O(r^{0}),$$
  

$$K_{r} = \sigma \sqrt{\pi l}, \quad K_{r} = \tau \sqrt{\pi l} \qquad (1)$$

$$2v(x,0) = [(\eta+1)/G]K_1\sqrt{|x/2\pi|} + O(x), \ x \le 0.$$
(2)

$$2u(x,0) = [(\eta+1)/G]K_{II}\sqrt{|x/2\pi|} + O(x), \ x \le 0.$$
(3)

Here  $\sigma_{\theta}(r,\theta)$  and  $\tau_{r\theta}(r,\theta)$  are normal and shear stresses, respectively,  $K_{I}$  and  $K_{II}$  are Stress Intensity Factors (SIFs) by I and II modes, respectively, 2v(x,0) is the opening of crack flanks, 2u(x,0) is the crack sliding displacement, G is the shear modulus,  $\eta = 3-4\mu$  for planar deformation,  $\eta = (3-\mu)/(1+\mu)$  for planar stress state, where  $\mu$  is the Poisson's ratio. It is appropriate to study planar deformation for crystals and for fine-grained solids, relations corresponding to planar stress state are used. The stress field, see relation (1) and Fig. 1, is defined in a single crystal solid, and the opening and displacement of crack flanks, see relation (2) and Fig. 1, is defined beyond a single crystal solid.

Let us consider the brittle-ductile transition caused by fracture of single crystals for sufficiently long cracks, more precisely,  $l > 10r_e$ , where  $r_e$  is the constant of atomic lattice. When restrictions are imposed on crack lengths 2l, relations (1)-(3) can be simplified: terms of the order  $O(r^0)$  are omitted in relation (1), and terms of the order O(x) are omitted in relations (2), (3). Further the Neuber-Novozhilov approach will be used for materials with the regular structure, for the specific linear size of isotropic single crystal, the constant of atomic lattice  $r_e$  is chosen. The averaging interval coincides with the segment length  $OO_1$  in Fig. 1, it is equal to  $r_e$  or  $2r_e$  for materials without damages.

## **3 STRENGTH AND DEFORMATION CRITERIA**

When stresses  $\sigma_{\rm m}$ ,  $\tau_{\rm m}$  gradually increase, proportional loading in the complicated stress state occurs in the vicinity of a crack tip. Crack branching (see Kornev and Kurguzov, 1999; Kornev and Kurguzov, 2000a; Kornev and Kurguzov, 2001) or dislocation emission is possible (see Kornev and Kurguzov, 2000). Branching takes place at every structural level of material as shown by Kornev (2000), and dislocation occurs only for the Nano-structure. The system chooses one or another way of branching that is associated with strength characteristics of the material. The curves of the theoretical strength of the Coulomb-Mohr type are given in Fig. 2 (see Macmillan, 1983; Paul, 1983) for two different material structures and the way of loading is pointed. The following notations are used in Fig. 2 for the imaginary plane  $\sigma - \tau$ :  $\sigma$  and  $\tau$  are normal and shear stresses, respectively, in the area under consideration in the complicated stress state when the symmetry axis of strength structure characteristics coincide with a crack-cut; curves 1 and 2 are curves of the theoretical strength of the first and second structures such that  $\sigma_m = \sigma_{m1} = \sigma_{m2}$ are theoretical (ideal) tensile strengths (see Macmillan, 1983; Paul, 1983), and  $\tau_{m1} \neq \tau_{m2}$  are theoretical (ideal) shear strengths (if theoretical tensile strengths of structures coincide, theoretical shear strengths are essentially different); the proportional loading way is figured by 3 beside the arrow. The way of loading relation is characterized by the following  $\sigma_{13}^* / \tau_{13}^* = \sigma_{23}^* / \tau_{23}^* = C_3 = \text{const}$  (notations  $\sigma^*, \tau^*$  are used for stresses of critical states with subscripts corresponding to the structure number and the type of loading); aside from the constant  $C_3$ , the loading way can be given by the angle  $\varphi$ . This constant  $C_3$  or the angle  $\varphi$  define the type of loading in the plane  $\sigma - \tau$ , the loading type being independent on strength characteristics of materials.

3.1 The strength criterion. Material with a structure containing a crack is under consideration. Let us assume that: i) the strength characteristics of this material possess a symmetry axis that coincides with the crack axis, ii) the material is defect-free. Kornev and Kurguzov (1999), Kornev and Kurguzov (2000a), Kornev and Kurguzov (2001), Kornev (2000) have been proposed the discrete-integral criterion of brittle strength of the Neuber-Novozhilov type for crack extension following the chosen directions  $\pm \theta$  that are defined by angles of branching, see Fig 1,

$$\left\langle \sigma_{\theta}(\theta) \right\rangle \leq \sigma^{*}, \left\langle \tau_{r\theta}(\theta) \right\rangle \leq \tau^{*}, \qquad (4)$$

$$\left\langle \sigma_{\theta}(\theta) \right\rangle = \frac{1}{nr_{e}} \int_{0}^{nr_{e}} \sigma_{\theta}(r,\theta) dr, \left\langle \tau_{r\theta}(\theta) \right\rangle = \frac{1}{nr_{e}} \int_{0}^{nr_{e}} \tau_{r\theta}(r,\theta) dr, \quad n = 1, 2.$$

Here  $\langle \sigma_{\theta}(\theta) \rangle$ ,  $\langle \tau_{r\theta}(\theta) \rangle$  are averaged normal and shear stresses in the chosen directions  $\pm \theta$ . At  $\langle \sigma_{\theta}(\theta) \rangle < \sigma^*$ ,  $\langle \tau_{r\theta}(\theta) \rangle < \tau^*$ , a crack does not extend (branching is absent). When averaged stresses  $\langle \sigma_{\theta}(\theta) \rangle$ ,  $\langle \tau_{r\theta}(\theta) \rangle$  coincide with stresses of critical states  $\sigma^*, \tau^*$ , the criterion (3) is satisfied: the following occur in the chosen directions  $\pm \theta^*$  (*i*) extension of a straight crack over the averaging interval if  $\theta^* = 0$  (branching is absent), (*ii*) crack propagation over the averaging interval when the crack of length 2*l* branches out if  $\theta^* \neq 0$ , see Fig. 1. When a crack has extended at  $\theta^* = 0$ , the criterion (4) is applied repeatedly to the straight crack of the length  $2(l + nr_e)$  for estimation of possibility for new crack branching. When branching takes place at  $\theta^* \neq 0$ , the stress field for a branched crack should be refined, see, for instance, the reference book by Savruk (1988) and Argatov and Nazarov (2002), as well as the references to them. Then the procedure of estimation of possibility for branching of a crack with fractures is repeated. However, at  $\theta^* \neq 0$  for a branched crack, the stress field is essentially complicated because the deformation mode II occurs along the mode I.

We estimate the type of stress state in the vicinity of a crack tip depending on the angle  $\theta$  ( $-\pi < \theta < \pi$ ). For I fracture mode, the results have been obtained by Kornev (2003), Kornev (2003a), Kornev (2004). For II fracture mode, we derive the distribution of stresses  $\sigma_{\theta}, \tau_{r\theta}$  by simplified relations (1) when terms of the order  $O(r^0)$  are omitted. For some angle  $\theta$ , the following relation can be written

 $\tau_{r\theta}(r,\theta)/\sigma_{\theta}(r,\theta) = \langle \tau_{r\theta}(\theta) \rangle / \langle \sigma_{\theta}(\theta) \rangle = (3\sin^2(\theta/2) - 1)/(3\sin(\theta/2)\cos(\theta/2)).$ (5)

Thus, simple shear  $\sigma_{\theta} \equiv 0, \tau_{r\theta} \neq 0$  is realized on the crack continuation  $\theta = 0$  in the vicinity of its tip; at  $\theta = -2 \arcsin(1/\sqrt{3})$ , simple tension  $\sigma_{\theta} > 0, \tau_{r\theta} \equiv 0$  is realized in the immediate vicinity of the tip crack; at arbitrary angles  $-\pi < \theta < \pi, \theta \neq 0, \theta \neq \pm 2 \arcsin(1/\sqrt{3})$ , the generalized stress state  $\sigma_{\theta} \neq 0, \tau_{r\theta} \neq 0$  takes place. The angle  $\theta = 2 \arcsin(1/\sqrt{3})$  is eliminated from consideration since simple compression on the imaginary plane  $\sigma - \tau$  corresponds to this angle, i.e.,  $\sigma_{\theta} < 0, \tau_{r\theta} \equiv 0$ .

When one of symmetry axes of a structure coincides with the cut, the limiting strength curve of the Coulomb-Mohr type in the plane  $\sigma - \tau$  is described by the function  $\rho(\varphi) = \rho(-\varphi) = f(\varphi) = f(-\varphi)$  (see Fig. 2 and Paul, 1968) that can be related to the Goldstein and Salganik (1974) principle of local symmetry for I fracture mode. It should be noted that all four quadrants on the imaginary plane  $\sigma - \tau$  are used for II fracture mode, the  $\varphi = \pm \pi$  angle is eliminated from consideration since simple compression on the imaginary plane  $\sigma - \tau$  corresponds to this angle. Principle of local is not valid for II mode.

Equations describing branching of inner cracks of the sliding mode take the form

$$\frac{2l(\theta)}{r_e} = \frac{nf^2(\varphi)}{\tau_{\infty}^2 \cos^2(\theta/2)[1+3\sin^2(\theta/2)]}, -\pi < \theta < \pi, \theta \neq 2 \arcsin\frac{1}{\sqrt{3}};$$
  
$$\varphi = \arctan\frac{3\sin^2(\theta/2) - 1}{3\sin(\theta/2)\cos(\theta/2)}, -\pi \le \theta \le 0; \ \varphi = \pi + \arctan\frac{3\sin^2(\theta/2) - 1}{3\sin(\theta/2)\cos(\theta/2)}, 0 \le \theta \le \pi.$$

By relations obtained, calculations for typical functions  $f(\varphi)$  were performed.

3.2 Kink of crack trajectories at the generalized stress state. The crack extension under plane loading and transverse shear corresponding to I and II fracture modes are under consideration. The relations have been obtained that describe the kinking angle of a crack trajectory for the arbitrary generalized stress state when curves of the theoretical strength of a single crystal of the Coulomb-Mohr type are known. A crack extends in the following directions: i) normally to the direction of greatest tension when there are no shear stresses in the vicinity of its tip (Erdogan-Sih hypothesis) and material behavior is brittle; ii) along the direction of maximum shear when there are no normal stresses in the vicinity of its tip and material behavior is ductile (emission of dislocations occurs); iii) along some direction corresponding to the generalized stress state when material behavior is quasi-brittle or quasi-ductile (either opening mode of interatomic bonds or dislocation emission for the generalized stress state occur).

*3.3 The deformation criterion for Nano-structures*. Deformation criteria have been described in works by Kornev (2003), Kornev (2003a), Kornev (2004), where the simplest model of Frenkel-Kontorova is used (see Kornev and Kurguzov, 1999; Kornev and Kurguzov, 2000a; Kornev and Kurguzov, 2001). For construction of deformation criteria, relations (2) and (3) are used.

## 4 CRACK BRANCHING, CRACK KINKING. ABOUT THE PRINCIPLE OF LOCAL SYMMETRY

The principle of the local symmetry is realized for I fracture mode in the vicinity of the crack tip if the crystal symmetry axis coincides with the crack axis, and the theoretical strength curve possesses the appropriate symmetry. When asymmetric perturbations of an atomic lattice occur in the vicinity of the crack tip or the symmetry axis of a single crystal is inconsistent with the crack axis, the principle of the local symmetry fails for I and II fracture modes.

The work was supported by Russian Foundation for Basic Research (Grant No. 04-01-00191), Integration Project of RAS No. 3.11.1, and Grant of Russian Federation President No. NSH -319. 2003.1.

## REFERENCES

I.I. Argatov and S.A. Nasarov, Energy release at crack kinking in a plane anisotropic solid, *Prikl, Matem. Mekhan.* [in Russian], **66**, No. 3, 502-514 (2002).

R.V. Goldstein and R.L. Salganik, Brittle fracture of solids with arbitrary crack, *Int. J. Fract.*, **10**, 507–523 (1974).

P. Gumbsch, An atomistic study of brittle fracture: Toward explicit failure criteria from atomistic modeling, *J. Mater. Res.*, **10**, No.11, 2897–2907 (1995).

A. Kelly, W.R. Tyson, and A.H. Cottrell, Ductile and brittle crystals, *The Philos. Mag.*, **15**, 567–586 (1967).

J.F. Knott, Mechanics of fracture. In: *R. Latanision and J.R.Pickens (eds.), Atomistics of Fracture,* Plenum Press, New York, 209–235, 1983.

V.M. Kornev, Integral criteria for the brittle strength of cracked bodies with defects in the presence of vacancies at the tip of a crack. Strength of compacted ceramic-type bodies, *J. Appl. Mech. and Techn. Phys.*, **37**, No.5, 756-764 (1996).

V.M. Kornev, Hierarchy of strength criteria of structured brittle media. Satellite initiation of microcracks, *J. Appl. Mech. and Techn. Phys.*, **41**, No. 2, 367-375 (2000).

V.M. Kornev, Branching and kink of opening crack paths in polycrystal, *Physical Mesomechanics*, [in Russian] **6**, No. 5, 37-46 (2003).

V.M. Kornev, Fracture of brittle and ductile crystals. Strength and deformation criteria, *Prikl, Matem. Mekhan*, [in Russian] **67**, No. 6, 1027-1039 (2003).

V.M. Kornev, Rupture crack branching in solids with structural hierarchy, *Int. J. of Fracture*, [to be published] (2004).

V.M. Kornev and V.D. Kurguzov, A discrete-integral strength criterion for complicated stress states, *Fatigue & Fracture of Engineering Materials & Structures*, **22**, No. 11, 989–995 (1999).

V.M. Kornev and V.D. Kurguzov, Modeling of an edge dislocation and estimate of the dislocation core for a closed-packed atomic layer, *J. Appl. Mech. and Techn. Phys.*, **41**, No. 5, 211-216 (2000).

V.M. Kornev and V.D. Kurguzov, The discrete-integral strength criterion for complicated stress state, *Izv. RAN, Mekhan. Tverd. Tela* [in Russian], No. 6, 99-106 (2000a).

V.M. Kornev and V.D. Kurguzov, The discrete-integral strength criterion for complicated stress state at the presence of foreign atoms, In: *Dinamica Sploshnoi Sredy, RAN Siberian Branch* [in Russian], Institute of Hydrodynamics, Issue 119, 62-67, 2001.

V.M. Kornev and Yu.V. Tikhomirov, Loss of stability of on atomic chain region in the presence of impurity. Strength reduction of cracked brittle solids, *J. Appl. Mech. and Techn. Phys.*, **37**, No. 3, 433-443 (2000).

N.H. Macmillan, The ideal strength of solids. In: *R. Latanision and J.R.Pickens (eds.), Atomistics of Fracture, Plenum Press, New York, 95–164, 1983.* 

G. Rauchs, D. Munz, and T. Fett, Calculation of crack tip phase transformation zones in TZP with the weight function method, *Fracture Mechanics of Ceramics. Ed. R. C. Bradt and all, Vol. 13. Crack–Microstructure Interaction, R–Curve Behavior, Environmental Effects in Fracture, and Standardization,* Kluwer Academic / Plenum Pulishers, New York, Boston, Dordrecht, London, Moscow, 1–8, 2002.

B. Paul, Macroscopic criteria for plastic flow and brittle fracture, *Fracture. An Avanced Treatise*. *Ed. H. Liebowitz, Vol. II. Mathematical Fundamentals,* Academic Press, New York, London, 313–496, 1968.

J.R. Rice, Dislocation nucleation from a crack tip: an analysis based on the Peierls concept, J. *Mech. Phys. Solids.*, **40**, No. 2, 239–271 (1992).

J. Rice and R. Thomson, Ductile versus brittle behavior of crystals, *The Philos. Mag.*, **29**, 73–97 (1974).

M.P. Savruk, Fracture mechanics and strength of materials, Vol. 2: Stress-intensity factor in cracked bodies [in Russian], Naukova Dumka, Kiev, 1988.

K.G. Schmitt-Thomas, *Metallkunde fur das Maschinenwesen*, Springer-Verlag, Berlin, Heidelberg, New York, 1989.

R. Thomson, Physics of fracture. In: *R. Latanision and J.R.Pickens (eds.), Atomistics of Fracture,* Plenum Press, New York, 167–204, 1983.