

**POTENTIAL ENERGY STATE DURING CRACK
PROPAGATION IN DISCRETE MODEL OF MATERIAL**

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Abstract. *The theory of fracture mechanics has two main approaches to the problem of crack propagation: the continuum mechanics, and the atomic approach. They are presented in classical literature of fracture mechanics listed in [3], [4], [5], [9], [10], [11], [15], [18] and [19]. Expecting that duality of approaches will be over passed by integrative theory in the future, this paper deals with the atomic approach of cracks inside a discrete model of material (atomic lattice). Solids may be represented as systems of discrete masses linked by interacting forces, interatomic forces or simple bonds. Not only mechanical loads are involved in crack growth, but also chemical, thermo-mechanical, electro-mechanical, acoustic and other physical phenomena are also involved. Ability of a discrete model to explain crack healing, slow subcritical crack growth, sound generation during crack propagation, effects of chemical processes at the tip of the crack, nonlinearity of stress, strain and energy distribution in the crack tip region, influence of temperature on crack propagation and gives great advantage to procedures based on model of discrete masses (atomic lattice). Two intrinsic interatomic force functions are used to represent mechanical interaction between the neighboring atoms (discrete masses) in lattice. Released potential energy, as a result of crack propagation through the lattice, by breaking interatomic bonds is presented. One- and two-dimensional models of lattice and relations for total potential energy of selected models of lattice are presented.*

Key words: *crack, mathematical form of localized energetic structure, discrete model of material, atomic lattice, functions of interatomic forces, potential energy of atomic bond, total potential energy of lattice, activation energy, strain energy surfaces.*

1. INTRODUCTION, FRAMEWORK

Fracture is a complex phenomenon caused by rupture of chemical bonds between the neighboring atoms. Many different sources of fracture exist. The beginning of the fracture can be caused by defects in the lattice, like the irregular position of the arbitrary atom in the lattice, or the absence of an atom in the lattice knot, or substituting of a one element atom by another (chemical element) atom. Bond force is defined as the differential with respect to distance between atoms of the function of the interatomic potential energy. Lattice of discrete model interferes with the free development of the crack and acts as a barrier to the crack development. One of the first discrete models was developed by Thomson, Hsieh, Rana and Fuller. Orowan (1949) and Gilman (1960) had already discussed single nonlinear crack-tip bond. If smaller and smaller elements of volume are considered, models of continuum based fracture mechanics are more and more inadequate. The introduction of discrete model and lattice spacing takes us closer to real physical structure of material, but mathematically, simplicity and generality of continuum mechanics are lost.

According to G. C. Sih [17]: "Classical thermodynamics and continuum mechanics have not been able to explain the irreversible nature of material behavior, simply because their formulations are based on oversimplifying and physically unrealistic assumptions." Locally, material elements can experience multiaxial stress and strains even though the remotely applied load is pure tension or compression [12-14]. On the other hand, it is shown that a great number of physical objects with localized energy are described theoretically with the same mathematical structure [1]: the energy is the sum of two terms (one is a nonconvex function of field variables and the other is quadratic function of their derivatives). From this arises a question about the mathematical form which has the possibility to describe the localized energy structures as regions of high field gradients. Such theory should be **nonlinear**. Following this, the **mathematical form of localized energetic structure** should be [1]:

$$E = \int_{-\infty}^{\infty} \left[F(u) + \frac{1}{2} \cdot \varepsilon^2 \cdot \left(\frac{du}{dx} \right)^2 \right] dx \quad (1)$$

where: $u(x)$ - is a scalar field, $F(u)$ - is the energy density (nonconvex).

In paper [1] the authors suggested that if we denote by $u(x)$ the relative displacements of atoms on both side of a sliding plane, the elastic energy of distortion is due to interaction of atoms along the sliding plane, and this is periodic function $\sin(2 \cdot \pi \cdot u/b)$ of displacement $u(x)$ with period b (b - is lattice parameter).

"On the other hand: the argument that whether matter is made of invisible atoms or of an underlying continuum has been debated, but still is not completely resolved in scientific terms. The possibility that the two opposite concepts of particle and field may not be mutually exclusive and may represent different aspects of the same reality is still open. The late Albert Einstein argued strongly against the coexistence of field and matter. He regarded matter as being constituted by the regions of space in which the **field is extremely intense** and believed **that field is the only reality**. (Sih G. C. [18])

2. INTRINSIC INTERATOMIC COHESIVE FORCES

One of the sources of crack-tip singularity in continuum linear elastic solutions is the application of Hooke's law beyond its limits of validity (see Figure 2 and 3). The simplicity of linear elastic fracture mechanics solutions provides useful physical insights into the nonlinear nature of crack initiation and propagation. Approximation of Hooke's law is replaced by sine function or by more accurate potential function to describe stress - strain or force - deformation function. Stress (force) separation function rise up to a maximum, as the crack tip approaches to atomic bond, and decrease asymptotically to zero, when atomic bond is broken. In this way, process of crack propagating can be described as a step by step breaking of atomic bonds, but at the same time as a continual process (described by continual functions). Before the atomic bond is completely broken (force of interatomic interaction is close to zero), next bonds along the chain are stretched (see Figures 12, 17 and equation 3). Propagation of the crack tip through the chain of atoms is connected with nonlinear response of the atomic bonds at the surrounding. Rheological models for corresponding materials can be used to represent the response of atomic bonds in the lattice of discrete material points as [6].

Gilman approximated the interatomic bond force-displacement function by a half-sine curve [10, 11]:

$$F_B(u) = F_{Th} \sin\left(\frac{2\pi u}{\delta'}\right) \quad (2u \leq \delta') \quad (2)$$

Interatomic forces are dependent on the type of bonding, and can be presented as related to interatomic distance b , by [10]:

$$F(b) = F_o \cdot \left[\left(\frac{b_o}{b}\right)^n - \left(\frac{b_o}{b}\right)^m \right] \quad (3)$$

where: n represents attractive forces (n is 2 for ionic bonding and $n=7$ for Van der Waal's bonding), m represents repulsive forces (for closed electron shells m can be 12), b_o is the spacing in atomic lattice on zero stress level (equilibrium lattice spacing) and b is the lattice spacing on some stress level.

If $(b - b_o)$ is equal to $2u$ (see Figure 12), we may write strain of atomic bond as: $\varepsilon_b = 2u/b_o$.

From the stand point of approximated forces of interatomic bonds which are given by equations (2) and (3) it is understandable why the maximum of σ_y [15] is shifted from the crack tip up to some distance (Figure 1). Atomic bonds behind σ_{max} on Figure 1 are stretched over maximum of interatomic force, and interatomic force is decreasing like it is shown in Figures 2, 3 and 4. Interatomic bonds are not broken at that region, but there is irreversible part of deformation and it looks like the crack tip as determined by forces is ahead of the crack tip as determined by the geometric contour.

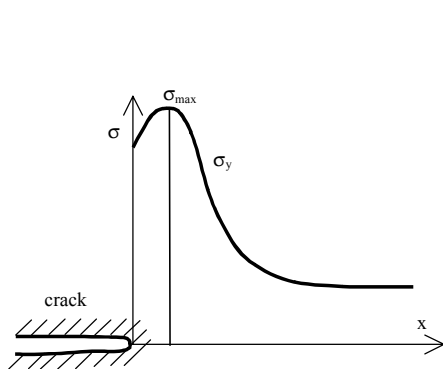


Fig. 1. Distribution of σ_y stress ahead of the crack tip [15].

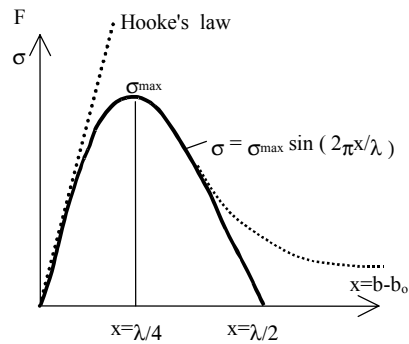


Fig. 2. Sine wave approximation of force (stress) function [10].

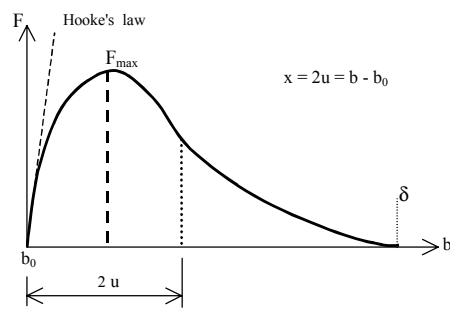


Fig. 3. Interatomic forces given by function in the form of relation (3).

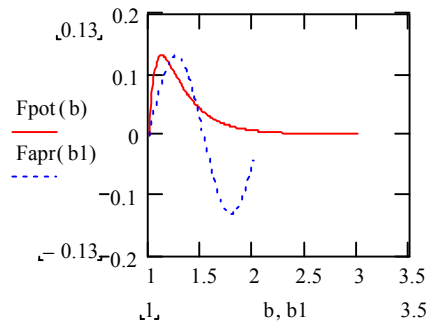


Fig. 4. Comparison of interatomic forces approximated by sine wave or by potential function

3. INTERATOMIC POTENTIAL ENERGY

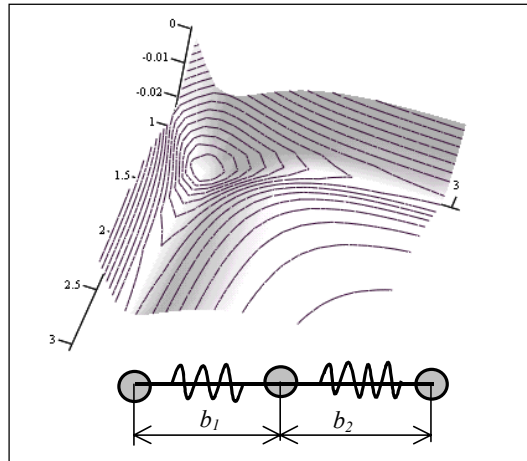
The cohesion energy for the separated crack-tip bond when the bonds are stretched up to the breaking displacement $2u_i$ is defined by:

$$U_{BB} = \int_0^\delta F_B(u_i) d(2u_i) \tag{4}$$

Let's consider a system of tree atoms or discrete material points conected with bonds. If we create a three dimensional surface, representing the potential energy of this system, low regions correspond to low potential energy, and high regions correspond to high levels of potential energy (shown in Fig. 5). Crack propagates from one valley to the another, through a saddle point between the crests of the hills of energy surface. The path of the crack trajectory from one valley of energy to the other is the activation path wich depends on the level of the activation energy. The system is stable at the bottom of the

valley. The height of the saddle point between two valleys is the level of activation energy needed to activate crack propagation or to break interatomic bond.

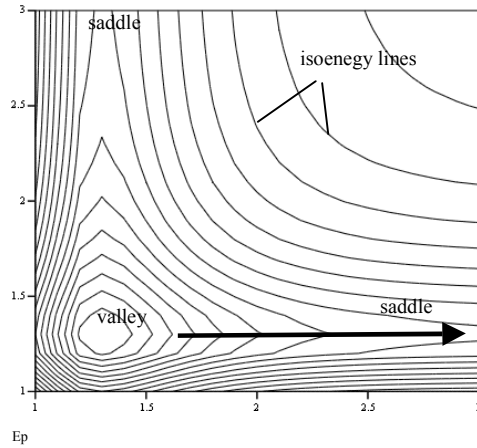
$$E_p(b_1, b_2) = \frac{1}{2} \left[\left(\frac{b_o}{b_1} \right)^m - \left(\frac{b_o}{b_1} \right)^n \right] \cdot (b_1 - b_o) + \frac{1}{2} \left[\left(\frac{b_o}{b_2} \right)^m - \left(\frac{b_o}{b_2} \right)^n \right] \cdot (b_2 - b_o) \quad (5)$$



Ep

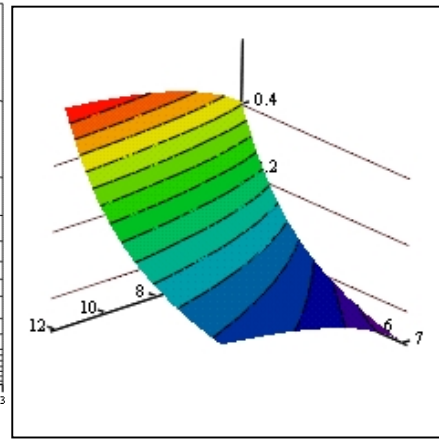
Fig. 5. Surface of potential energy for system of three atoms bonded by atomic interaction

Influence of potentials m and n on the value of potential energy of an atomic bond is shown on Figure 7. Values of m are changing from 5 to 12 and values of n are changing from 2 to 7.



Ep

Fig. 6. Isoenergy lines projected on x-y plane for system of three atoms bonded by atomic interaction



U_{bond}

Fig. 7. Surface of potential energy depending on value of m and n

4. DISLOCATION OF ATOMS IN TWO AND THREE DIMENSIONAL LATTICE

It is shown that the interatomic force is directly related to the interatomic distance. Displacement of one atom in lattice causes changes of distances between neighbouring atoms. Further, changing of interatomic distances from zero equilibrium configuration (assumption that interatomic forces are equal to zero) in the lattice, to some new equilibrium configuration, when forces in atomic bonds are different from zero, cause change of the interatomic forces and the interatomic potential energy. Changes of distances between the knots in lattice cause changes of volume as well as changes of directions (angle between atomic bonds) and this generates new shape of lattice (see Figures 8, 9 and 17).

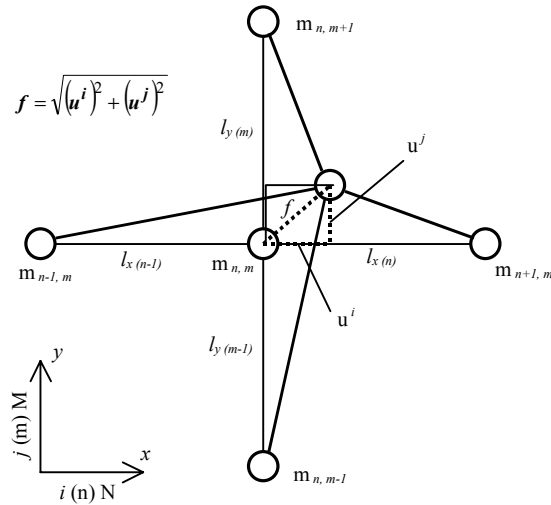


Fig. 8. Dislocation of atom in two-dimensional lattice.

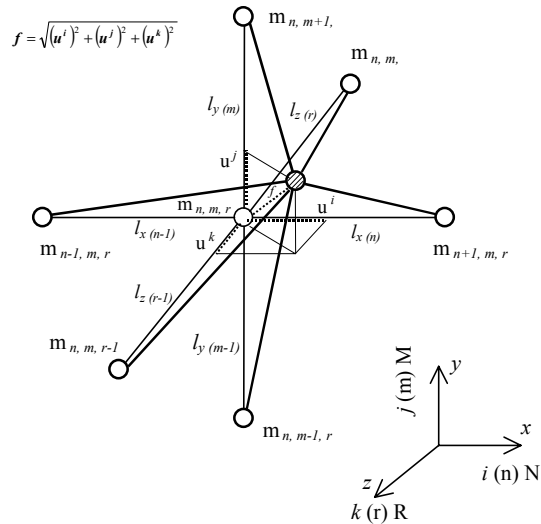


Fig. 9. Dislocation of atom in three-dimensional lattice

According to Figure 8, absolute deformations Δl_x and Δl_y of atomic bonds in x and y direction, for two-dimensional lattice are given by the following relations

$$\Delta l_{x(n-1)} = l'_{x(n-1)} - l_{x(n-1)} = \left(\sqrt{(l_{x(n-1)} + u^i)^2 + (u^j)^2} \right) - l_{x(n-1)} \quad (6)$$

$$\Delta l_{x(n)} = l'_{x(n)} - l_{x(n)} = \left(\sqrt{(l_{x(n)} - u^i)^2 + (u^j)^2} \right) - l_{x(n)} \quad (7)$$

$$\Delta l_{y(m-1)} = l'_{y(m-1)} - l_{y(m-1)} = \left(\sqrt{(l_{y(m-1)} + u^j)^2 + (u^i)^2} \right) - l_{y(m-1)} \quad (8)$$

$$\Delta l_{y(m)} = l'_{y(m)} - l_{y(m)} = \left(\sqrt{(l_{y(m)} - u^j)^2 + (u^i)^2} \right) - l_{y(m)} \quad (9)$$

According to Figure 9, absolute deformations Δl_x , Δl_y and Δl_z , of atomic bonds in x and y direction, for three-dimensional lattice are given by the following relations

$$\Delta l_{y(m-1)} = l'_{y(m-1)} - l_{y(m-1)} = \sqrt{(l_{y(m-1)} + u_{nmr}^j)^2 + (u_{nmr}^i)^2 + (u_{nmr}^k)^2} - l_{y(m-1)} \quad (10)$$

$$\Delta l_{y(m)} = l'_{y(m)} - l_{y(m)} = \sqrt{(l_{y(m)} - u_{nmr}^j)^2 + (u_{nmr}^i)^2 + (u_{nmr}^k)^2} - l_{y(m)} \quad (11)$$

$$\Delta l_{x(n-1)} = l'_{x(n-1)} - l_{x(n-1)} = \sqrt{(l_{x(n-1)} + u_{nmr}^i)^2 + (u_{nmr}^j)^2 + (u_{nmr}^k)^2} - l_{x(n-1)} \quad (12)$$

$$\Delta l_{x(n)} = l'_{x(n)} - l_{x(n)} = \sqrt{(l_{x(n)} - u_{nmr}^i)^2 + (u_{nmr}^j)^2 + (u_{nmr}^k)^2} - l_{x(n)} \quad (13)$$

$$\Delta l_{z(r-1)} = l'_{z(r-1)} - l_{z(r-1)} = \sqrt{(l_{z(r-1)} + u_{nmr}^k)^2 + (u_{nmr}^i)^2 + (u_{nmr}^j)^2} - l_{z(r-1)} \quad (14)$$

$$\Delta l_{z(r)} = l'_{z(r)} - l_{z(r)} = \sqrt{(l_{z(r)} - u_{nmr}^k)^2 + (u_{nmr}^i)^2 + (u_{nmr}^j)^2} - l_{z(r)} \quad (15)$$

5. TOTAL POTENTIAL ENERGY OF THE SYSTEM

If we consider a pair of atoms, we can draw a curve to represent a force of interatomic interaction, as well as a curve to represent the energy of their interaction as a function of interatomic distance. The released strain energy U in relation (16) is equal to the area under the F -curve in Figure 3. The released strain energy U in relation (18) is equal to the area under the F -curve in Figure 2. For the force-displacement function given by relations (2) and (3), by using relations (4), we get the released potential energies given by equations (17), and (19). Graphical visualization of the released potential energy for both assumed force - displacement functions are presented in Figures 10 and 11.

$$U = \int_{b_o}^{\delta} F(b) db = \int_{b_o}^{\delta} F_o \left[\left(\frac{b_o}{b} \right)^n - \left(\frac{b_o}{b} \right)^m \right] db \quad (16)$$

$$U = F_o \cdot \delta \cdot \frac{(b_o^m \cdot n \cdot \delta^n - b_o^m \cdot \delta^n + b_o^n \cdot \delta^m - b_o^n \cdot m \cdot \delta^m)}{(m-1) \cdot (n-1) \cdot \delta^m \cdot \delta^n} - F_o \cdot b_o \cdot \frac{(n-m)}{(m-1) \cdot (n-1)} \quad (17)$$

$$U = \int_{b_o}^{\delta} F(b) db = \int_{b_o}^{\delta} F_{Th} \cdot \sin\left(2 \cdot \pi \cdot \frac{b-b_o}{\delta}\right) db \tag{18}$$

$$U = \frac{1}{2 \cdot \pi} \cdot \delta \cdot F_{Th} \left[1 - \left(2 \cdot \cos^2\left(\pi \cdot \frac{b_o}{\delta}\right) - 1 \right) \right] \tag{19}$$

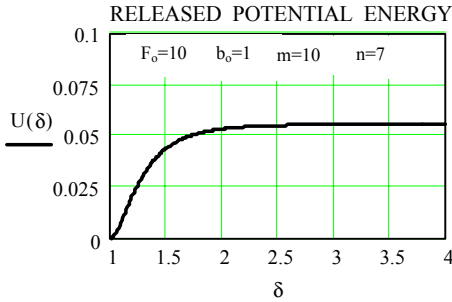


Fig. 10. Released potential energy for force assumed by function (3)

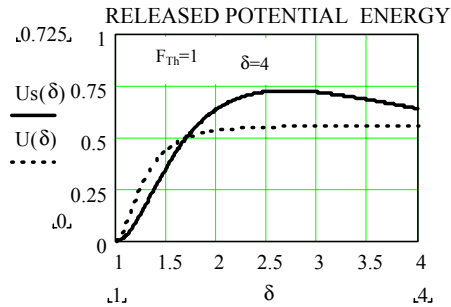


Fig. 11. Released potential energy for force assumed by sine function (2) (solid line), compared with function (3) (dotted line)

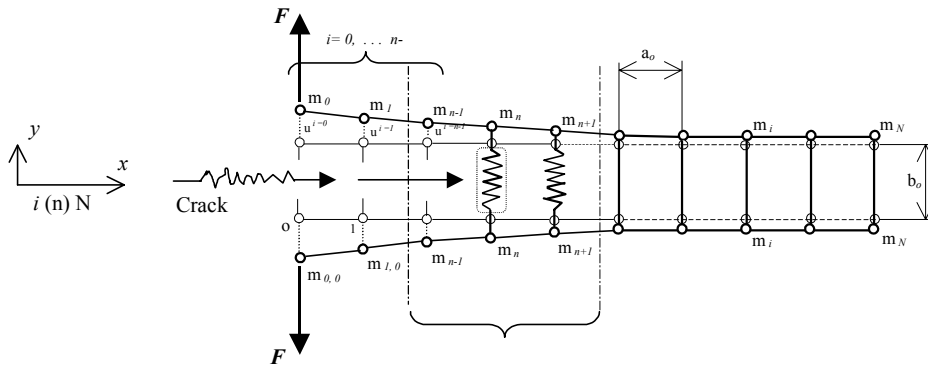


Fig. 12. One-dimensional model of lattice and crack propagating through the chain of atoms [11]

The total potential energy of the lattice presented in Figure 12 may be written as a function of displacements u_j of atoms along the chain [11]. The first term in relation (20) is the energy of the nonlinear strained bond in front of crack tip. The second term in relation (20) is the released potential energy of broken bonds behind the crack tip. The third term is the strain energy of stretchable elements ahead of the crack tip. The fourth is the strain energy is potential energy of applied loading system.

$$U = U_B(u_n) + n \cdot U_{BB} + \frac{1}{2} \cdot c_y \cdot \sum_{i=n+1}^{\infty} (2 \cdot u_j)^2 + c_{xy} \cdot \sum_{i=1}^{\infty} (u_{i+1} - 2 \cdot u_i + u_{i-1})^2 + 2 \cdot F \cdot u_o \tag{20}$$

where: c_y, c_{xy} - rigidity of atomic bonds (y - direction and bending, respectively), and:

$$U_{BB} = \int_0^{\delta} F_B(u_i) d(2 \cdot u_i) \tag{21}$$

The released strain energy U_{BB} in relation (21) is equal to the area under the F-curve on Figures 2 and 3. For force-displacement function given by relations (2) and (3), by using relations (4), we are getting released potential energies given by equations (16), (17), (18) and (19). Released potential energy for both assumed force displacement functions are presented on Figures 10 and 11.

Continual motion of crack tip through one-dimensional model of lattice (see Figures 12) may be described by relation (22) (Lawn B. [11]) and its graphic is presented in Figure 13.

$$U(z) = a_o \cdot \left((-G^* + 2 \cdot \gamma_B) \cdot z + \left(\frac{\Gamma_B \cdot a_o}{\pi} \right) \cdot \sin\left(\frac{2 \cdot \pi \cdot z}{a_o} \right) \right) \tag{22}$$

where: a_o is the interatomic distance, G^* is the rate of released mechanical energy, Γ_B - is the lattice-trapping modulation factor in cohesion energy, γ_B - is the intrinsic surface energy of solid body, Γ_B, γ_B are material quantities).

If we assume that the potential energy of atomic two-dimensional cubic lattice is distributed according to the sine law:

$$U(x, y) = a \sin \left[\left(\frac{1}{c} \right) \cdot \sqrt{R^2 - |a \cdot (\sin(x))^2 + b \cdot (\sin(y))^2|} \right] \tag{23}$$

we get the surface of potential energy shown on Figure 14, 15, and 16. Shape of potential energy surface depends on prescribed parameters a, b and c in assumed function.

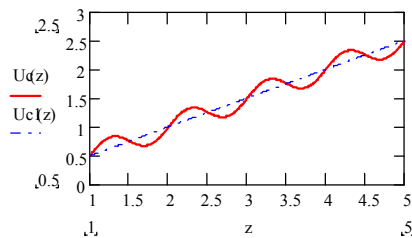


Fig. 13. Potential energy function during crack propagation through one-dimensional atomic chain (Fig. 12)

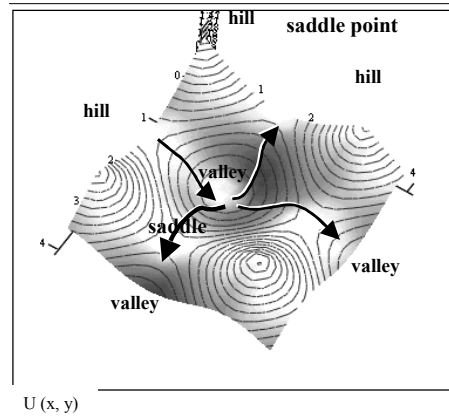
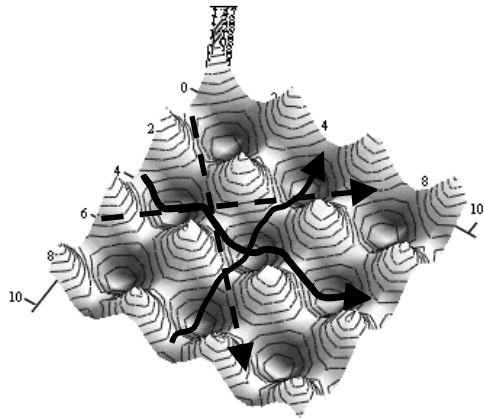


Fig. 14. Surface of potential energy for two-dimensional x-y lattice and possible trajectories of crack propagation through a saddle points

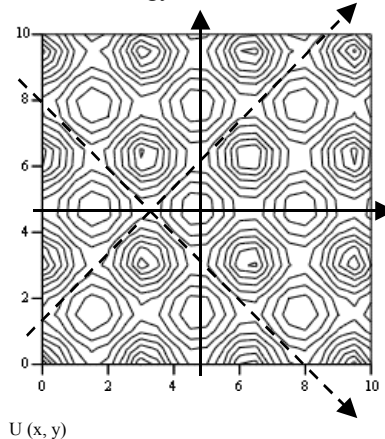
To produce crack growth for one step, available activation energy must be higher than height between the bottom of the valley and saddle point. Sources of activation energy are mechanical waves, fluctuation of thermal energy, and random changes of interatomic

distances caused by vibrations of atoms around their geometric locations (equilibrium positions) and external loading conditions. When external load is applied in this way that the atomic distances are increased up to the critical level, the force rises up to a maximum and the activation energy is high enough to overpass the crest of the saddle point. In the case when the breaking of atomic bonds supplies enough energy for the next step of crack propagation (breaking next bond or overpassing next saddle point), the crack continues to propagate without external sources of energy (see Figures 13, 14, 15, and 16). Randomly distributed, varying kinetic energy is in fact the thermal energy, and local fluctuation of interatomic distance is connected with fluctuation of thermal energy.



U(x,y)

Fig. 15. Surface of potential energy for two-dimensional x-y lattice and possible trajectories of crack propagation



U(x, y)

Fig. 16. Projection (x-y) of potential energy surface and possible directions of crack propagation

The total potential energy of the system of material points (two-dimensional lattice shown on Figure 17) may be written as a function of displacements u^j and released potential energy of broken atomic bonds as

$$U_o = U_n(u_n) + n \cdot U_V + \frac{1}{2} \cdot c_y \cdot \sum_{i=n+1}^N (2 \cdot u_{i,o}^j)^2 + \sum_{i=1}^N 2 \cdot \left(\frac{1}{2} \cdot c_{xy} (u_{i+1,o}^j - 2 \cdot u_{i,o}^j + u_{i-1,o}^j)^2 \right) - 2 \cdot \sum_{i=0}^N F_i' \cdot u_{iM} \quad (24)$$

$$U_1 = \frac{1}{2} \cdot c_y \cdot \sum_{i=0}^N (u_{i1}^j - u_{i0}^j)^2 + \sum_{i=1}^N \left(\frac{1}{2} \cdot c_{xy} (u_{i+11}^j - 2 \cdot u_{i1}^j + u_{i-11}^j)^2 \right) \quad (25)$$

$$U_m = \frac{1}{2} \cdot c_y \cdot \sum_{i=0}^N (u_{im}^j - u_{i,m-1}^j)^2 + \sum_{i=1}^N \left(\frac{1}{2} \cdot c_{xy} (u_{i+1m}^j - 2 \cdot u_{im}^j + u_{i-1m}^j)^2 \right) \quad (26)$$

$$U_M = \frac{1}{2} \cdot c_y \cdot \sum_{i=0}^N (u_{iM}^j - u_{i,M-1}^j)^2 + \sum_{i=1}^N \left(\frac{1}{2} \cdot c_{xy} (u_{i+1M}^j - 2 \cdot u_{iM}^j + u_{i-1M}^j)^2 \right) \quad (27)$$

Total potential energy of two-dimensional lattice is:

$$U_{TOT} = \sum_{j=0}^M U_j = U_o + 2 \cdot \sum_{i=1}^{M-1} U_i + 2 \cdot U_M \tag{28}$$

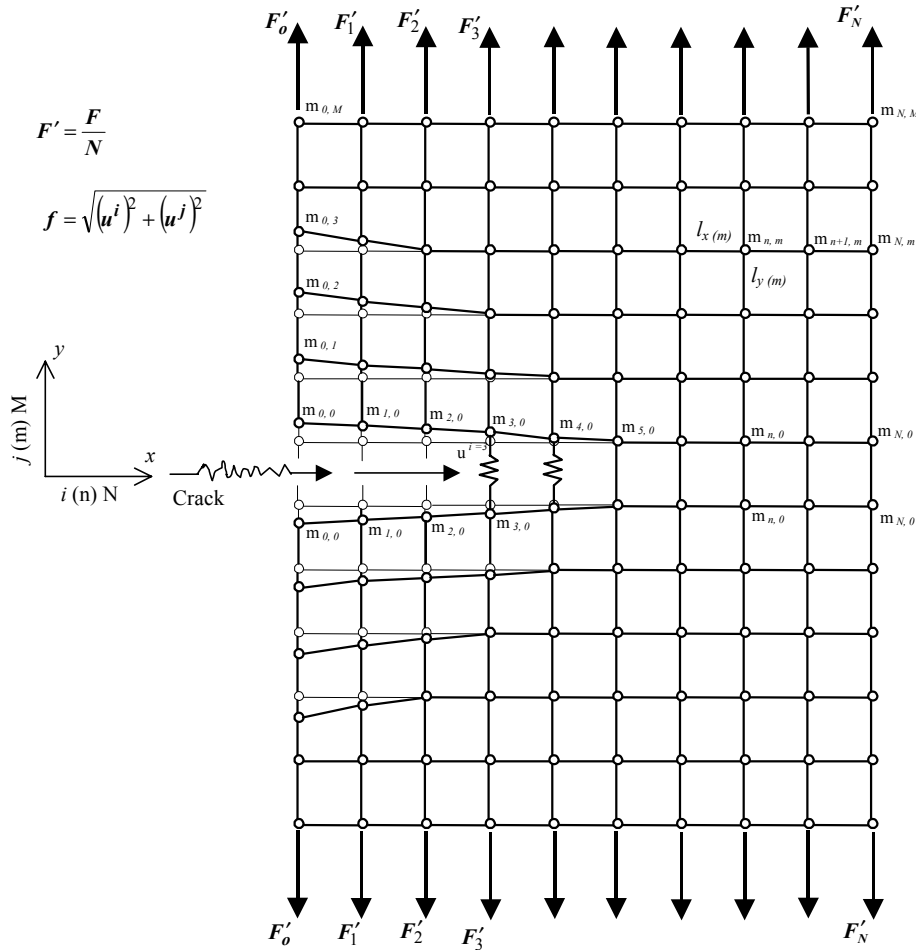


Fig. 17. Model of two-dimensional lattice

Research done in references [12], [13] and [14] (on macroscopic level and by using FEM) indicated that the influence of crack on the distribution of strain (deformation) energy is limited over relatively short distances.

The surface of the specific strain energy $A_{def} = f(x,y)$ for plane $z=0$ is presented in Fig. 19. It can be seen from Fig. 19 that redistribution of deformation energy resulted with high energy on crack front, where the "mountain of energy" has a peak. On the other hand, there is a valley, with an energy level lower than the general (or global) energy level $\bar{A}_{def} = 1$. The bottom of the valley has $\bar{A}_{def} = 0.185$. It is visible in Fig. 19 that distribution of strain energy resulted with high value of energy in front of crack tip,

where the peak of energy stored in material exists. It can be seen from Fig. 18 that the specific deformation (strain) energy increases from the middle plane $z=0$ to the front and back free surface of the plate, and that peaks of energy are close to free surfaces of the plate.

Regions of the plate further from the crack remain undisturbed and deformation energy is clearly constant. Also, the stress state at a distance higher than one plate thickness is evidently two-dimensional, and the stresses are independent of the thickness coordinate. This gives us the opportunity to draw the conclusion that the influence of the crack is local and the rest of the plate stays “undisturbed”. This analysis suggests that analytical solutions should be locally three-dimensional.

The derivation that the peak of energy is located not just on the edge of the crack, but on some distance [14], coincides with the conclusions driven from the atomic (discrete) model of material (see Figures 1, 2, and 3).

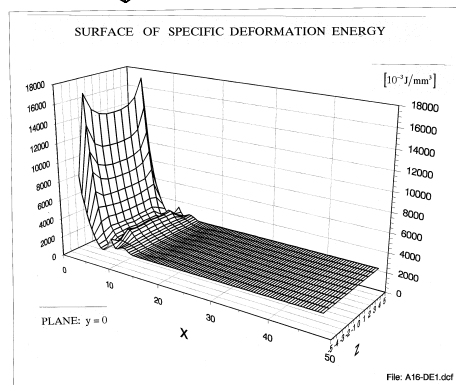
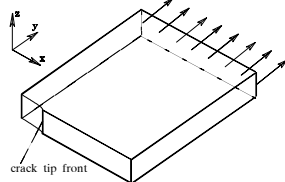


Fig. 18. Reconstructed surface of the specific deformation (strain) energy $A_{def} = f(x,y)$ for plane $y = 0$. (Ref. [14])

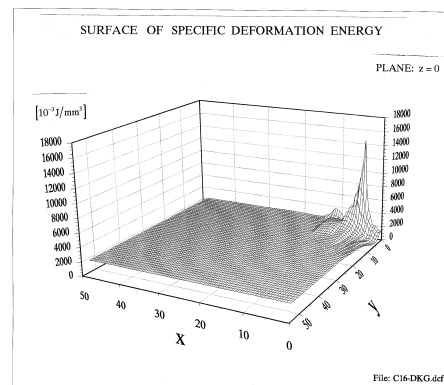


Fig. 19. Reconstructed surface of the specific deformation (strain) energy $A_{def} = f(x,y)$ for plane $z = 0$. (Ref. [14])

6. CONCLUSIONS

Interactions of different physical phenomenon involved in initiation and propagation of cracks, and in the process of fracture and damage, have directed research towards analyzing processes at atomic and molecular level. Capability of modern experimental equipment gives the opportunity to record data about values and processes at atomic level. A synthesis and a short review of the results produced by the researchers listed in the references of the present paper, and some results of author are given. There is consistency between conclusions based on discrete (atomic) and macroscopic models, related to potential energy distribution in vicinity of the crack tip. Two assumed

functions of interatomic forces are presented and their relation with the potential energy is analyzed. It is shown that: ***The site of fracture coincides with the location of minimum strain energy density, and yielding with maximum strain energy density*** (Sih G. C., see Ref. [17]).

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STANJE POTENCIJALNE ENERGIJE U TOKU NAPREDOVANJA PRSLINE U DISKRETNOM MODELU MATERIJALA

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Teorija mehanike loma ima dva osnovna pristupa problemu napredovanja prsline:

- mehanika kontinuuma i*
- atomistički pristup.*

Oni su prikazani u klasičnoj literaturi mehanike loma [3], [4], [5], [9], [10], [11], [15], [18], [19]. Očekujući da će dualnost ovih pristupa biti prevaziđena integrativnom teorijom mehanike loma u budućnosti, ovaj rad se bavi atomističkim stanovištem. Atomistički pristup razmatra prsline unutar diskretnog modela materijala (atomska mreža). Čvrsta tela se mogu prikazati kao sistemi diskretnih masa povezanih silama uzajamnog dejstva, međuatomskim silama ili jednostavno (vezama). Nisu samo mehanička opterećenja uključena u rast prsline, već takođe hemijske, termo-mehaničke, elektro-mehaničke, zvučne i druge fizičke pojave. Sposobnost diskretnog modela da objasni zarastanje prsline, spori podkritični rast prsline, stvaranje zvuka u toku napredovanja prsline, uticaje hemijskih procesa na vrh prsline, nelinearnost rasporeda napona, deformacija i energije u oblasti vrha prsline, uticaj temperature na napredovanje prsline, daje veliku prednost postupcima zasnovanim na modelu diskretnih masa (atomska mreža).

Dve svojstvene funkcije međuatomskih sila su korišćene da prekažu mehaničku interakciju između susednih atoma (diskretnih masa) u mreži. Prikazana je oslobođena potencijalna energija kidanjem međuatomskih veza, kao posledica napredovanja prsline kroz mrežu. Prikazani su jedno dimenzionalan i dvodimenzionalan model mreže i relacije za totalnu potencijalnu energiju izabranih modela mreže.

Ključne reči: prsline, matematička forma lokalizovane energetske strukture, diskretni model materijala, atomska mreža, funkcije međuatomskih sila, potencijalna energija atomske veze, totalna potencijalna energija mreže, energija aktiviranja, površine energije deformacije.