Crack and fracture theory of liquid crystals and quasicrystals

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Abstract Liquid crystals and quasicrystals are fascinating phases of modern physics and chemistry, they are also important materials in current and potential applications. The liquid crystals belong to intermediate phase between fluids and solids in macroscopic sense, they present behaviour of anisotropic fluids, i.e., they behave both characters of conventional fluids and anisotropic elastic solids. The quasicrystals present unusual mechanical and physical properties due to the atomic arrangement being quite different from that of conventional crystals. To describe the mechanical behaviour of quasicrystals, one must introduce two different displacement fields, this leads to two different strain tensors and two stress tensors. This paper reports some results in the study on crack and fracture problems of liquid crystals and quasicrystals. The nonlinear fracture analysis is important for the both materials. However there is fundamental difficulty in the analysis due to lack of plastic constitutive equations for them. Some physical models and relevant mathematical methods are developed to overcome the difficulty, and some results have been obtained, which are of a development of fracture theory of conventional structural materials.

Keywords Liquid crystals, quasicrystal, crack, fracture

1. Introduction

Liquid crystals, in macroscopic sense, are anisotropic fluids. Therefore they belong to an intermediate phase between fluids and crystals. The mechanical behaviour of liquid crystals presents the character of both fluids and solids.

There are various types of liquid crystals, here we discuss the mechanics only for nematic, smectic and columnar liquid crystals.

Different from the behaviour of both fluids and solids, the deformation and motio of liquid crystals should be introduced a vector named director $\mathrm{n}=\left(n_x,n_y,n_z\right)$ apart from displacement vector $\mathrm{u}=\left(u_x,u_y,u_z\right)$ and velocity vector $V=\left(V_x,V_y,V_z\right)$.In addition, the constitutive equation of liquid crystals is different from either generalized Newton’s equation or generalized Hooke’s equation. For example, for the nematic liquid crystals, we have constitutive law [1]

$$\sigma_{ij} = \sigma_{ij}^0 + \sigma_{ij}^{'}$$
$$\sigma_{ij}^0 = -\Pi_{ik} \frac{\partial}{\partial x_j} n_k , \Pi_{ik} = \frac{\partial F}{\partial \left(\frac{\partial}{\partial x_i} n_k \right)} \tag{1}$$
$$\sigma_{ij}^{'} = -p\delta_{ij} + \mu \frac{1}{2} \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right)$$

in which F is the free energy of the system, n_k the component of the director mentioned above, p the pressure, μ the fluid viscosity, V_i the component of velocity and δ_{ij} the unit tensor, respectively. The free energy consists of three parts: first one arising from bulk deformation (by the displacements), second one arising from deformation due to curvature, another arising from the coupling between distortion and curvature, i.e.,

$$F = F_e + F_c + F_{ec} \tag{2}$$

where

$$F_e = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \tag{3}$$

denotes the conventional elastic strain energy, or the Cauchy strain energy, C_{ijkl} the elastic constants, ε_{ij} the Cauchy strain tensor, and

$$F_c = \frac{1}{2} K_1 (div(\mathbf{n}))^2 + \frac{1}{2} K_2 (\mathbf{n} \cdot rot\mathbf{n}))^2 + \frac{1}{2} K_3 (\mathbf{n} \times rot\mathbf{n}))^2 \tag{4}$$

the Frank energy due the curvature, and K_1, K_2, K_3 the modulia of Frank deformation, in addition

$F_{ec} =$ Deformation energy of coupling between Cauchy strain and Frank strain (5)

For the most cases F_{ec} can be omitted.

The equations of motion include the equations of momentum conservation,

$$\rho \left[\frac{\partial V_i}{\partial t} + (\mathrm{V} \cdot \nabla V_i) \right] = \frac{\partial \sigma_{ij}}{\partial x_j} \tag{6}$$

equation of mass conservation

$$\frac{\partial \rho}{\partial t} + div(\rho \mathrm{V}) = 0 \tag{7}$$

and equation of entropy conservation if there is no dissipation

$$\frac{\partial S}{\partial t} + div(S\mathrm{V}) = 0 \tag{8}$$

where ρ denotes the mass density of the matter, S the entropy. If there is dissipation the equation (8) should be changed, but the discussion is omitted here. From the above simple introduction, we can mind that the equations of the liquid crystals are quite complicated. Some detail for the solutions will be introduced later.

For smectic liquid crystals, the director stands for

$$\mathrm{n} = \left(\frac{\partial u_z}{\partial x}, \frac{\partial u_z}{\partial y}, 1 \right) \tag{9}$$

where u_z is the displacement component in the direction normal to the layers of smectics, and $u_x = u_y = 0$.

For columnar liquid crystals, the director stands for

$$\mathrm{n} = \left(\frac{\partial u_x}{\partial z}, \frac{\partial u_y}{\partial z}, 1 \right) \tag{10}$$

where u_x, u_y are the displacement components along the directions x, y respectively, and $u_z = 0$.

Quasicrystals belong to another fascinating phase of condensed matter, first observed in 1982[2]. Macroscopically their main feature is that there are two different displacement fields, one is the phonon field u, according to the terminology of physics, which is similar to the displacement field in the classical elasticity under the long-wave length approximation, the other is the phason field which is new concept out of the regime of the classical continuum mechanics. The introducing of the phason field results in a great challenge to the traditional continuum mechanics. This leads to two different strain tensors, one is the Cauchy strain tensor

$$\varepsilon_{ij} = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{11}$$

another is the phason strain

$$w_{ij} = \frac{\partial w_i}{\partial x_j} \tag{12}$$

The constitutive equations are

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} + R_{ijkl}w_{kl} \qquad H_{ij} = R_{klij}\varepsilon_{kl} + K_{ijkl}w_{kl} \tag{13}$$

in which σ_{ij} is the stress tensor associated with strain tensor ε_{ij}, H_{ij} the stress tensor associated with the strain tensor w_{ij}, C_{ijkl} the phonon elastic constants, K_{ijkl} the phason elastic constants, and R_{ijkl} the phonon-phason coupling elastic constants, respectively.

The equations of motion are as follows [39,40]

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} \tag{14}$$

$$\kappa \frac{\partial w_i}{\partial t} = \frac{\partial H_{ij}}{\partial x_j} \tag{15}$$

where $\kappa = 1/\Gamma_w$, in which Γ_w the dissipation kinematics coefficient of phason field of the material defined by Lubensky et al [3]. It is evident that the equation (14) represents the wave propagation, while equation (15) represents diffusion. Because σ_{ij} and H_{ij} are coupled, the motion of quasicrystals is in coupled of wave propagation and diffusion.

The above equations are only an outlook of dynamics of liquid crystals and quasicrystals, this reveals that the mechanics of either liquid crystals or quasicrystalsis quite different from that of conventional fluids as well as elastic solids (or periodic crystals), so the solutions of them are quite different from those of classical fluid dynamics and elasticity.

2. Crack and fracture of liquid crystals

The mechanics of liquid crystals are studied by de Gennes et al [4], Oswald et al [5] etc, the main attention of theirs was paid to discuss the dislocation and disclination problems, but there are some questions of the classical solutions which may be paradoxes, this suggests that the mechanics of liquid crystals needs to develop further. Brostow et al [5] started to study the crack problems in polymer liquid crystals. Because liquid crystals including nematic, smectic and columnar ones, they can be classified as monomer liquid crystals (MLCs) irrespectively of the fact whether they can or cannot polymerize into polymer liquid crystals (PLCs) [6]. That classification is due to Samuski [7] and has been used by a number of authors [8, 9]. The present model applies to MLCs and nematic, smectic and columnar phase LCs in particular. For studying crack problems of liquid crystals one must develop mechanics of liquid crystals, including three-dimensional elasticity, plasticity and dynamics.

The problem of screw dislocation in smectic liquid crystals A or smectics A for simplicity is a longstanding puzzle, de Gennes [4], Kleman [10], Pershan [11] and Landau and Lifscitz [12] presented the solution, but which may be of mistake. Pleineer [13] pointed out the problem of the solution, but the mistake could not be corrected. This problem shows in the theoretical system of mechanics of liquid crystals there may be some difficulties, in which the incompatibility between governing equations and boundary conditions is one of puzzles. For example, in the smectics A, the final governing equation is if only analyzing dislocation

$$\left(\rho B' \frac{\partial^2}{\partial z^2} - K_1 \nabla^2 \nabla^2\right) u_z = 0 \tag{16}$$

which is a partial differential equation of fourth order, which needs two boundary conditions to determine solutions, but the authors of Refs [4,10-13] gave only one boundary condition, this leads to the incompatibility between governing equation and boundary conditions and is the reason of their mistakes. Fan and Li [14] develop the elasticity of the smectic liquid crystals, pay attention to create the well-conditional boundary value problem of governing equation of mechanics of liquid crystals. So that Fan and Li give a correct solution for the dislocation problem as

$$u_z = \frac{b}{2\pi}\left[1 + D_1 r \sin\theta\right]\theta \tag{17}$$

in which

$$D_1 = \frac{-\frac{8}{3}\pi\alpha}{\left(R_0 + r_0\right)\left(\frac{\pi}{4}\alpha\beta + \frac{b^2 K_1}{8\pi}\right)\ln\frac{R_0}{r_0} + \frac{\pi}{320}\alpha\gamma\left(R_0 - r_0\right)} \tag{18}$$

where

$$\alpha = \left(\frac{b}{2\pi}\right)^4 \rho_0 B', \beta = 2 + \frac{32\pi^2}{3}, \gamma = 75 - 160\pi^2 + 256\pi^4 \tag{19}$$

in equations (15) and (19), $\rho_0 B'$ represents the Young's modulus in direction z of the smectics A, the meaning of K_1 is one of Frank modulus mentioned above, b the magnitude of the Burgers vector of dislocation, r_0 the size of dislocation core, R_0 the size of the body containing the dislocation. The solution (17) modifies the mistake of the classical solution of de Gennes-Kleman-Pershan.

The well-conditional boundary value problem just can develop the work on crack in liquid crystals. As an example, a solution of plastic crack in one of smenctics A is found by Fan [15] based on the dislocation pile-up concept, the size of plastic zone around crack tip and crack tip opening displacement are determined, shown in Figs. 1 and 2.

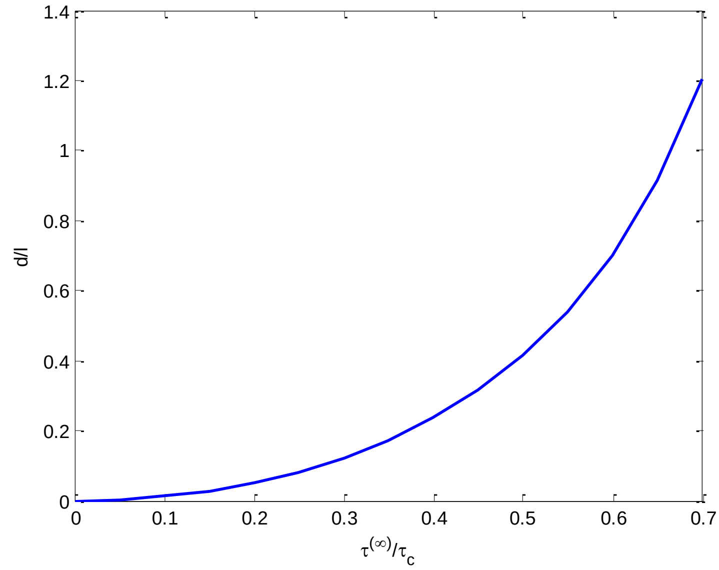

Fig.1 Variation of normalized plastic zone size with normalized applied stress

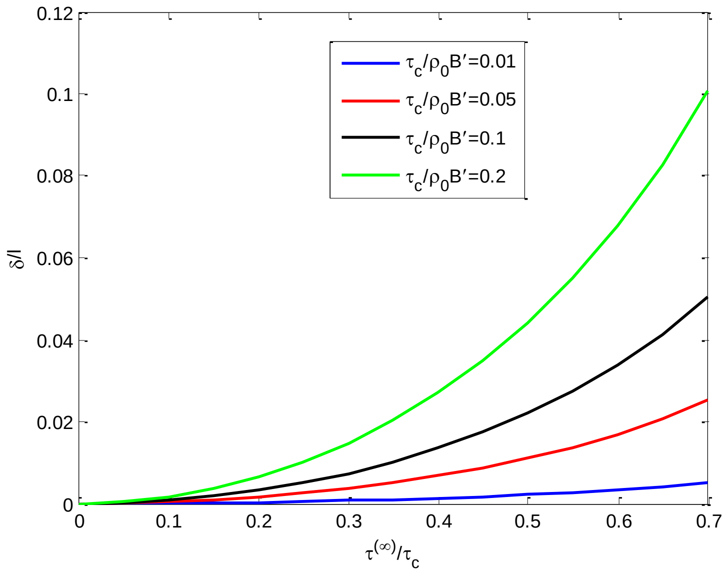

Fig.2 The variation of normalized crack tip opening displacement versus normalized applied stress

Other solutions for plastic crack in smectic A are obtained by Fan [16]. The three-dimensional elasticity of smectics B liquid crystals is studied by Fan [17], the governing equations are reduced to three generalized harmonic equations, and an elliptic disc-shaped crack problem is solved, an approximate analytic solution is constructed. Fan and Chen [18] studied the solution of plastic crack of columnar liquid crystals, but the result is more complicated than those of smectic liquid crystals A.

Due to the unusual structure of stress field of liquid crystals leads to some difficulties of the crack problem, for example, in the smectics A

$$\sigma_{\boldsymbol{xx}} = \sigma_{\boldsymbol{yy}} = \boldsymbol{K}_1 \nabla^2 \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{z}}, \sigma_{\boldsymbol{zz}} = \rho_0 \boldsymbol{B}' \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{z}}, \sigma_{\boldsymbol{zx}} = \sigma_{\boldsymbol{xz}} = -\boldsymbol{K}_1 \nabla^2 \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}$$

$$\sigma_{\boldsymbol{zy}} = \sigma_{\boldsymbol{yz}} = -\boldsymbol{K}_1 \nabla^2 \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{y}}, \sigma_{\boldsymbol{xy}} = \sigma_{\boldsymbol{yx}} = 0$$

it is evident that between the stress components the stress singularities will be quite different .

Due to the space limitation, we do not list the other questions and other results on mechanics of liquid crystals.

3. Linear theory crack and fracture of quasicrystals

The mechanics of quasicrystals is developed by many scientists, in which the elasticity of the material is advanced for example, refer to Lubensky et al [3], Ding et al [19], Fan and Mai [20], Fan [21]. The systematical mathematical theory of elasticity of quasicrystals is developed by Chinese group [21]. The elasticity, plasticity and dynamics of icosahedral quasicrystals, the most important class of the material, are well studied in the work. By introducing displacement potential, the plane elasticity of icosahedral quaiscrystals is reduced to solve the sextuple harmonic equation [21,22,23]

$$\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2 F(x,y) = 0 \tag{20}$$

From the equation we obtain the solution of a crack in icosahedral Al-Pd-Mn quasicrystals by the complex analysis of the Fourier analysis, which is given as follows

$$K_I^{\parallel} = \sqrt{\pi a}\, p \tag{21}$$

$$G_I = \frac{1}{2}\frac{\partial}{\partial a}[2\int_{-a}^{a}(\sigma_{yy}(x,0) \oplus H(x,0))(u_y(x,0) \oplus w_y(x,0))dx] = \frac{1}{2}(\frac{1}{\lambda+\mu} + \frac{c_7}{c_3})(K_I^{\parallel})^2$$

in which

$$c_3 = \mu(K_1 - K_2) - R^2 - \frac{(\mu K_2 - R^2)^2}{\mu K_1 - 2R^2}, c_7 = \frac{c_3 K_1 + 2c_1 R}{\mu K_1 - 2R^2}$$

$$c_1 = \frac{R(2K_2 - K_1)(\mu K_1 + \mu K_2 - 3R^2)}{2(\mu K_1 - 2R^2)}$$

The Fig. 3 shows the energy release rate variation and comparison between solutions of quasicrystals and crystals.

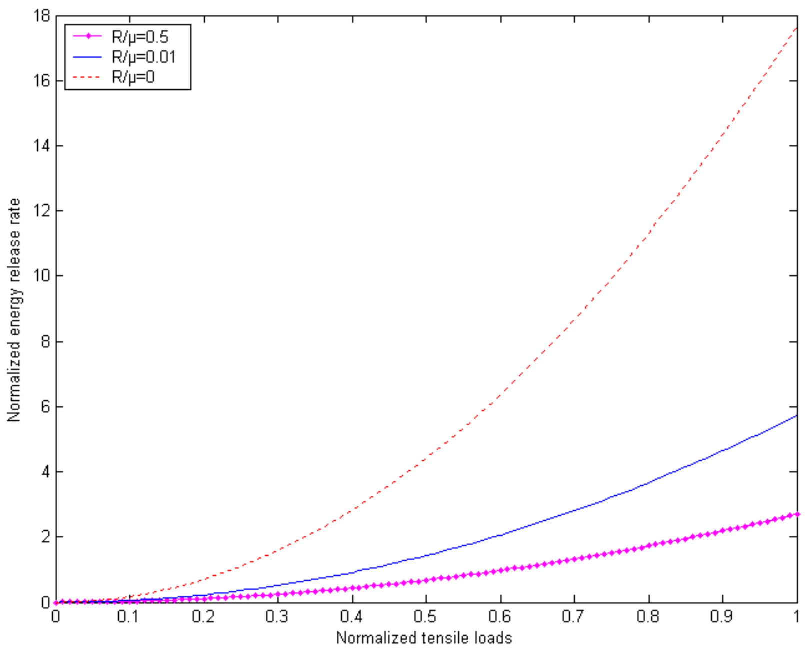

Fig.3 Influence of phason and phonon-phason coupling to the energy release rate

in which solution for crystals is also given. One can find that the solutions of quasicrystals and crystals are quite different each other (one corresponding to crystals is the case $R/\mu=0$).

Other solutions can be found in Ref [21].

4. Nonlinear solutions of cracks of quasicrystals

Though there are people try to give some explanations on plastic deformation by using dislocation model and so on, the problem is substantively unsolved so far. Due to lack of enough experimental data in macroscopy, the constitutive equation of plasticity of quasicrystals has not been set up. This leads to difficulty doing stress analysis of the material. One can say that the study is in an infant stage. In spite of these difficulties, people pay effort to do some work as above pointed out, the experiments[24-33] reported in the above references provide some hints, which are beneficial for the stress analysis for plasticity and defects of the material. In the following some semi-phenomenological and semi-theoretical results are listed, they may provide a reference for the researchers in the community.

4.1 Generalized cohesive force model [34,35]

Due to lack of constitutive equation of plasticity of quasicrystals up to now, it may be a possible way that we draw the results of classical plasticity, classical dislocation theory and classical nonlinear fracture theory to study some relevant problems in quasicrystals. A useful model in classical elasto-plastic fracture theory is so-called Dugdale-Barenblatt model, the paper [34] extended it to plastic analysis of quasicrystals, and named it be generalized Dugdale-Barenblatt model, the classical work has been done by [34] and [35]. In terms of the model, we determined the size of plastic zone around the crack tip of anti-plane problem of three-dimensional icosahedral quasicrystals

$$\delta_I = \lim_{x\to l} 2u_y(x,0) = \lim_{\varphi\to\varphi_2} 2u_y(x,0) = 2\left(\frac{1}{\lambda+\mu} + \frac{c_4}{c_2}\right)\cdot\frac{\sigma_s a}{\pi}\cdot\ln\sec\left(\frac{\pi}{2}\frac{p}{\sigma_s}\right) \qquad (22)$$

where

$$c_2 = \mu(K_1 - K_2) - R^2 - \frac{(\mu K_2 - R^2)^2}{\mu K_1 - 2R^2}, \quad c_4 = c_1 R + \frac{1}{2}c_2\left(K_1 + \frac{\mu K_1 - 2R^2}{\lambda+\mu}\right) \qquad (23)$$

and

$$c_1 = \frac{R(2K_2 - K_1)(\mu K_1 + \mu K_2 - 3R^2)}{2(\mu K_1 - 2R^2)}$$

The curve drawn from（22）refer to Fig.4，which shows the effect of phason and phonon-phason coupling is significant.

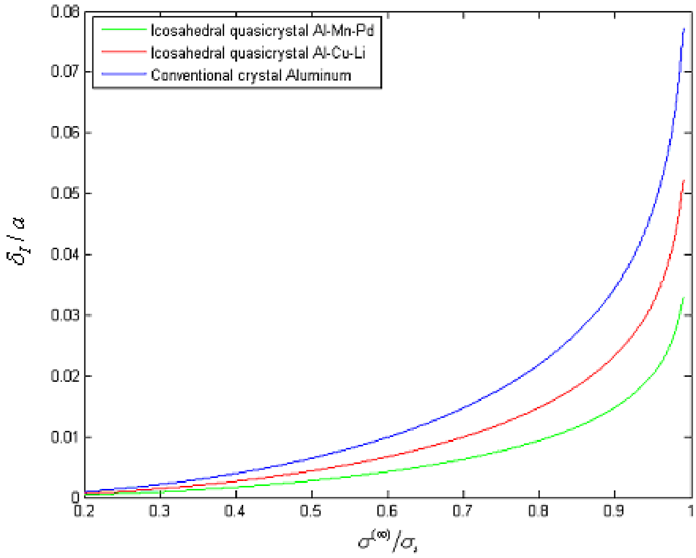

Fig. 4 Crack tip opening displacement versus applied stress for icosahedral quasicrystal [21]

4.2 Generalized continuum dislocations model [36]

We developed the continuous dislocation model [36], the results are identical to those given in Subsection 4.1.

4.3 Model based on generalized Eshelby energy-momentum tensor [37]

The generalized Dugdale-Barenblatt model and generalized continuum dislocation model, are quite different physically and mathematically, yield amazingly the complete identical solutions, we realized that there exist some inherent connection between the two models. Paper [37] gave a probe for the question. They proposed the generalized energy-momentum tensor of quasicrystals

$$G = Fn_1 - \sigma_{ij} n_j \frac{\partial u_i}{\partial x_1} - H_{ij} n_j \frac{\partial w_j}{\partial x_1} \tag{24}$$

and generalized integral of path independency

$$E = \int_{\Gamma} G d\Gamma \tag{25}$$

and found that they are the uniformly theoretical base of generalized Dugdale-Barenblatt model and generalized continuum dislocations model.The idea comes from the classical work of Eshelby [38] for crystals.

5. Dynamic solutions of cracks of quasicrystals

In the dynamic regime, the essential differences between phonons and phasons just can be profoundly revealed. However the problem presents fundamental difficulty because the mechanism of phason dynamics is not so clear so far.

Rocal and Lorman[39]and Fan et al [40], suggested the dynamic equation set for quasicrystals (14) and (15).This is the simplest dynamic equation set of quasicrystals, which coupled deformation geometry equations and stress-strain relations and lead to.the final governing equations of elasto-dynamics (or call elasto-/hydro-dynamics)

$$\left.\begin{aligned}
&\frac{\partial^2 u_x}{\partial t^2} + \theta \frac{\partial u_x}{\partial t} = c_1^2 \frac{\partial^2 u_x}{\partial x^2} + (c_1^2 - c_2^2)\frac{\partial^2 u_y}{\partial x \partial y} + c_2^2 \frac{\partial^2 u_x}{\partial y^2} + c_3^2\left(\frac{\partial^2 w_x}{\partial x^2} + 2\frac{\partial^2 w_y}{\partial x \partial y} - \frac{\partial^2 w_x}{\partial y^2}\right)\\
&\frac{\partial^2 u_y}{\partial t^2} + \theta \frac{\partial u_y}{\partial t} = c_2^2 \frac{\partial^2 u_y}{\partial x^2} + (c_1^2 - c_2^2)\frac{\partial^2 u_x}{\partial x \partial y} + c_1^2 \frac{\partial^2 u_y}{\partial y^2} + c_3^2\left(\frac{\partial^2 w_y}{\partial x^2} - 2\frac{\partial^2 w_x}{\partial x \partial y} - \frac{\partial^2 w_y}{\partial y^2}\right)\\
&\frac{\partial^2 u_z}{\partial t^2} + \theta \frac{\partial u_z}{\partial t} = c_2^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)u_z + c_3^2\left(\frac{\partial^2 w_x}{\partial x^2} - \frac{\partial^2 w_x}{\partial y^2} - 2\frac{\partial^2 w_y}{\partial x \partial y} + \frac{\partial^2 w_z}{\partial x^2} + \frac{\partial^2 w_z}{\partial y^2}\right)\\
&\frac{\partial w_x}{\partial t} + \theta w_x = d_1\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)w_x + d_2\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\right)w_z + d_3\left(\frac{\partial^2 u_x}{\partial x^2} - 2\frac{\partial^2 u_y}{\partial x \partial y} - \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_z}{\partial x^2} - \frac{\partial^2 u_z}{\partial y^2}\right)\\
&\frac{\partial w_y}{\partial t} + \theta w_y = d_1\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)w_y - d_2\frac{\partial^2 w_z}{\partial x \partial y} + d_3\left(\frac{\partial^2 u_y}{\partial x^2} + 2\frac{\partial^2 u_x}{\partial x \partial y} - \frac{\partial^2 u_y}{\partial y^2} - 2\frac{\partial^2 u_z}{\partial x \partial y}\right)\\
&\frac{\partial w_z}{\partial t} + \theta w_z = (d_1 - d_2)\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)w_z + d_2\left(\frac{\partial^2 w_x}{\partial x^2} - \frac{\partial^2 w_x}{\partial y^2} - 2\frac{\partial^2 w_y}{\partial x \partial y}\right) + d_3\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)u_z
\end{aligned}\right\} \tag{26}$$

where

$$c_1 = \sqrt{\frac{\lambda + 2\mu}{\rho}}, c_2 = \sqrt{\frac{\mu}{\rho}}, c_3 = \sqrt{\frac{R}{\rho}}, d_1 = \frac{K_1}{\kappa},\ \mathrm{d}_2 = \frac{K_2}{\kappa}, d_3 = \frac{R}{\kappa} \tag{27}$$

Note that c_1, c_2 and c_3 represent speeds of elastic waves, while d_1, d_2 and d_3 are not wave speeds, which are diffusive coefficients of phasons.

The numerical analysis is given for the specimen shown in Fig.5 made of icosahedral quasicrystal. After finite difference treatment on equation set (26) and corresponding boundary and initial conditions, the dynamic stress intensity factor for initiation of crack growth is obtained and shown in Fig.6.In the computation this is a simplest equation set of hydrodynamics of quasicrystals, which is simplified from the equations of Lubensky et al [3].

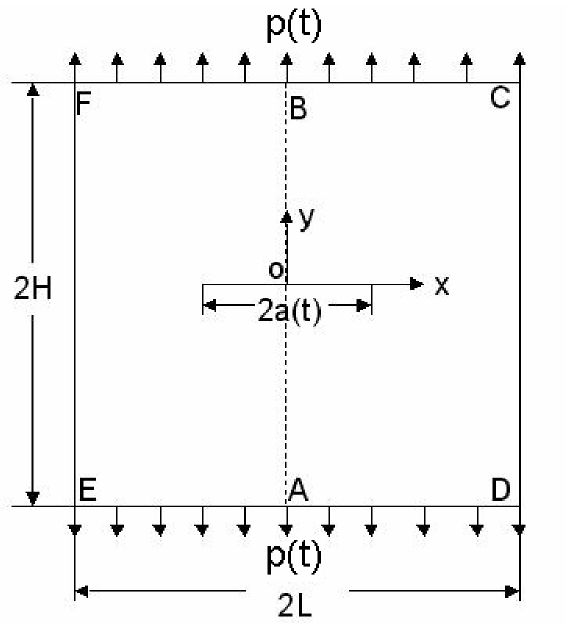

Figure 5 Sample containing a dynamic crack of two-dimensional quasicrystals

After finite difference treatment on equation set (26) and corresponding boundary and initial conditions, the dynamic stress intensity factor for initiation of crack growth is obtained and shown in Fig.6. In the computation

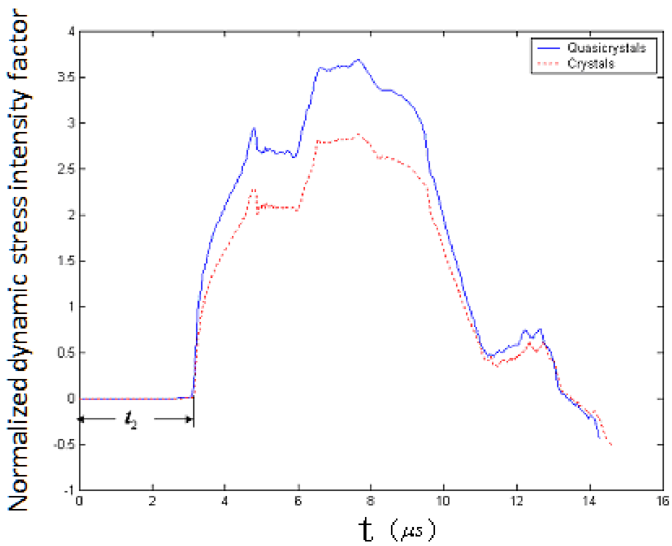

Figure 6 The dynamic stress intensity factor of rectangular specimen with a central crack of icosahedral Al-Pd-Mn quasicrystal under impact loading (for stationary crack)

the material is icosahedral Al-Pd-Mn quasicrystal with material constants：

$$\rho = 5.1\mathrm{g/cm}^3, \lambda = 74.2, \mu = 70.4(GPa), K_1 = 72, K_2 = -37(MPa)$$

$$\Gamma_w = 1/\kappa = 4.8\times10^{-19}\mathrm{m}^3\text{•}\mathrm{s/kg}=4.8\times10^{-10} cm^3\text{•}\mu s/g$$

$R/\mu = 0.01$ for quasicrystal, and $R/\mu = 0$ for crystal. It is evident that the results between quasicrystal and crystal are quite large.

The dynamic stress intensity factor for fast crack propagation of the central specimen is illustrated in Fig.7, which comes from monograph [21].

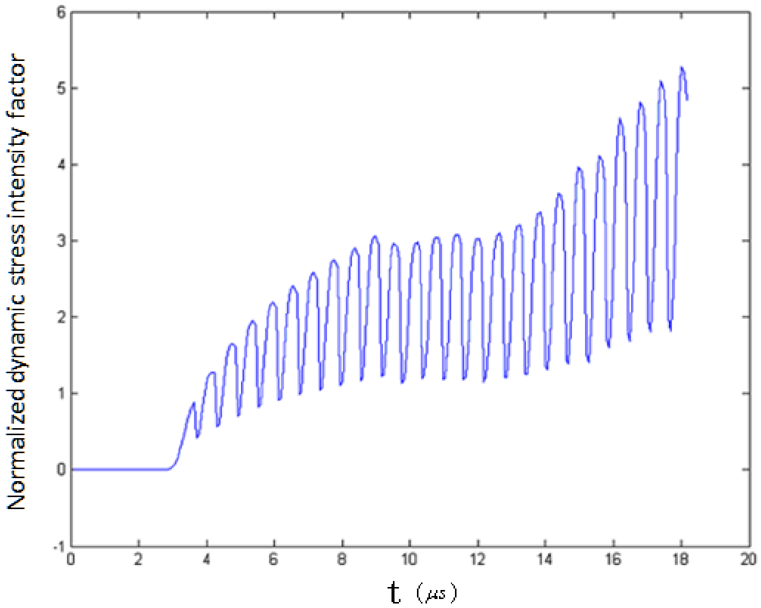

Figure 7 Dynamic stress intensity factor versus time of fast propagating crack in rectangular specimen with a central crack of icosahedral Al-Pd- Mn quasicrystal

The oscillation of the curve comes from the interference and reflection of waves, in which there are reasons come from numerical computation, it is needed doing further study.

6. Discussion and conclusion

The study of crack and fracture problems in liquid crystals is just begun, so it is in infant stage. The difficulty comes from some basic problems in the mechanics of liquid crystals, this also provides opportunity to gain the achievements in the field.

The linear elastic fracture theory of quasicrystals has been developed, the study of nonlinear and dynamic fracture theories of quasicrystals is also carried out, but faces some fundamental difficulties.

Because of many unsolved critical issues, the study is a fascinating research area of the materials science.

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