Vol 18 No 2, February 2009
1674-1056/2009/18(02)/0709-06

Chinese Physics B

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Dynamic behaviour of the icosahedral Al–Pd–Mn quasicrystal with a Griffith crack*

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(Received 23 May 2008; revised manuscript received 21 August 2008)

The dynamic response of an icosahedral Al–Pd–Mn quasicrystal with a Griffith crack to impact loading is investigated in this paper. The elastohydrodynamic model for the wave propagation and diffusion together with their interaction is adopted. Numerical results of stress, displacement and dynamic stress intensity factors are obtained by using the finite difference method. The effects of wave propagation, diffusion and phonon–phason coupling on the quasicrystal in the dynamic process are discussed in detail, where the phason dynamics is explored particularly.

Keywords: icosahedral quasicrystals, dynamic response, phason dynamics
PACC: 6200, 6220M, 6220D, 6140M, 6230

1. Introduction

Since the quasicrystal was first observed by Shechtman *et al*,[1] it has attracted extensive attention of numerous experimental and theoretical researchers. The mechanical behaviours, especially elasticity and defects of the new solid phase, play an important role in these studies. The fundamental challenge to the traditional continuum mechanics is the discovery of the new intra-variable phason field. This leads to two strain tensors and so two stress tensors; one is in the physical space or the parallel space, and the other is in the complement space or vertical space. Though the generalized static elasticity theory[2,3] is accepted by most scholars, it does not hold true for the elastohydrodynamics. For example, Bak[4] and Lubensky *et al* [5,6] presented two different viewpoints about it. We notice that these two arguments follow both the deformation geometry equation and generalized Hooke's law, and that the difference between them lies in the equations of motion. Ding *et al*,[7] Fan,[8] Li and Liu[9,10] followed Bak's arguments in their studies, that is, both phonon and phason were described as the wave propagation, i.e.

$$\rho\frac{\partial^2 u_i}{\partial t^2}=\frac{\partial \sigma_{ij}}{\partial x_j} \tag{1}$$

and

$$\rho\frac{\partial^2 w_i}{\partial t^2}=\frac{\partial H_{ij}}{\partial x_j}. \tag{2}$$

According to the arguments of Lubensky *et al* [5,6] and Fan *et al*,[11] the phason mode in quasicrystals corresponds to atomic jumps or diffusion, and there exists no conservation law corresponding to the diffusion of atoms, so we have the equations of motion

$$\rho\frac{\partial^2 u_i}{\partial t^2}=\frac{\partial \sigma_{ij}}{\partial x_j} \tag{3}$$

and

$$\kappa\frac{\partial w_i}{\partial t}=\frac{\partial H_{ij}}{\partial x_j}, \tag{4}$$

in which

$$\kappa=\frac{1}{\Gamma_w}$$

with Γ_w denoting the kinetic coefficient of phason field. The model accords with the experiment.[12] If we take the version of Eqs.(3) and (4), then dynamics for quasicrystals is different from the classical continuum dynamics at all, which, however, can bring some new insights into the continuum medium dynamics.

Among 200 quasicrystals that have been observed to date, there are 96 icosahedral quasicrystals, which play a central role in materials of this kind. The physical configuration considered in the present paper is an icosahedral quasicrystal containing a Griffith crack. Under the appropriate initial-boundary conditions,

*Project supported by the National Natural Science Foundation of China (Grant Nos 10672022 and 10372016).
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the equation set including the elasto-hydrodynamic equations, deformation geometry equations and generalized Hooke's law are solved by using the finite difference method. Numerical results of its dynamic response are given here in the present paper.

2. Elasto-hydrodynamic equations and initial-boundary conditions for icosahedral quasicrystals

According to quasicrystal elasticity theory,[7] we have the equations of deformation geometry

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

and

$$w_{ij} = \frac{\partial w_i}{\partial x_j}, \tag{5}$$

and the generalized Hooke's law

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} + R_{ijkl}w_{kl},$$

and

$$H_{ij} = R_{klij}\varepsilon_{kl} + K_{ijkl}w_{kl}, \tag{6}$$

where ε_{ij} and w_{ij} are the phonon strain and the phason strain, u_i and w_i are the phonon displacement and phason displacement, σ_{ij} and w_{ij} are the phonon stress component and the phason stress component, C_{ijkl}, K_{ijkl} and R_{ijkl} are the phonon, phason, phonon–phason coupling elastic constants respectively.

From Eqs.(3) and (4), and expressions (5) and (6), we obtain the governing equations of displacement as follows:

$$\begin{aligned}
&\frac{\partial^2 u_x}{\partial t^2} = 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} = 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} = 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} = 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} = d_1\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)w_y - 2d_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} = (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} \tag{7}$$

in which

$$\begin{aligned}
&c_1 = \sqrt{\frac{\lambda + 2\mu}{\rho}},\quad c_2 = \sqrt{\frac{\mu}{\rho}},\quad c_3 = \sqrt{\frac{R}{\rho}},\\
&d_1 = \frac{K_1}{\kappa},\quad d_2 = \frac{K_2}{\kappa}\quad \text{and}\quad d_3 = \frac{R}{\kappa}.
\end{aligned} \tag{8}$$

Note that c_1, c_2 and c_3 represent elastic wave speeds, d_1, d_2 and d_3 are diffusive coefficients.

Consider an icosahedral quasicrystal containing a Griffith crack subjected to a uniform dynamic load $P(t) = pf(t)$, where $f(t)$ is taken as the Heaviside function as shown in Fig.1, and assume that the crack penetrates through the z axis i.e. $\partial/\partial z = 0$.

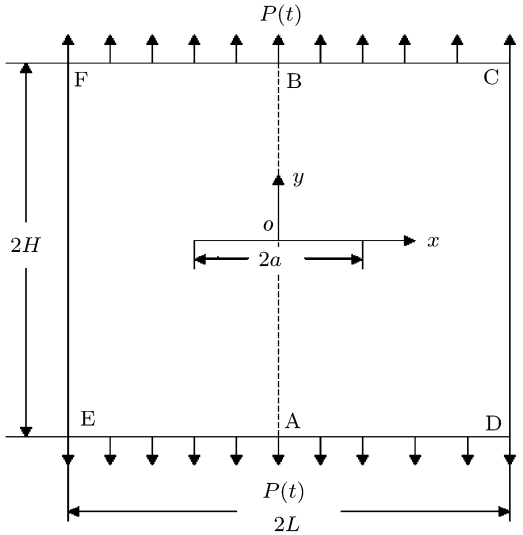


Fig.1. The specimen at rest or with crack propagating.

By examining the upper right part, the following boundary conditions should be satisfied:

$$
\begin{aligned}
&u_x = 0,\ \sigma_{xy} = 0,\ \ \sigma_{xz} = 0,\ \ w_x = 0,\ \ H_{xy} = 0,\ \ \text{and}\ \ H_{xz} = 0\ \ \text{on}\ \ x = 0\ \ \text{for}\ \ 0 \le y \le H;\\
&\sigma_{xx} = 0,\ \ \sigma_{xy} = 0,\ \ \sigma_{xz} = 0,\ \ H_{xx} = 0,\ \ H_{xy} = 0,\ \ \text{and}\ \ H_{xz} = 0\ \ \text{on}\ \ x = L\ \ \text{for}\ \ 0 \le y \le H;\\
&\sigma_{yy} = P(t),\ \ \sigma_{yx} = 0,\ \ \sigma_{yz} = 0,\ \ H_{yy} = 0,\ \ H_{yx} = 0,\ \ \text{and}\ \ H_{yz} = 0\ \ \text{on}\ \ y = H\\
&\text{for}\ \ 0 \le x \le L;\\
&\sigma_{yy} = 0,\ \ \sigma_{yx} = 0,\ \ \sigma_{yz} = 0,\ \ H_{yy} = 0,\ \ H_{yx} = 0,\ \ \text{and}\ \ H_{yz} = 0\ \ \text{on}\ \ y = 0\\
&\text{for}\ \ 0 \le x \le a;\\
&\text{and}\\
&u_y = 0,\ \ \sigma_{yx} = 0,\ \ \sigma_{yz} = 0,\ \ w_y = 0,\ \ H_{yx} = 0,\ \ \text{and}\ \ H_{yz} = 0\ \ \text{on}\ \ y = 0\\
&\text{for}\ \ a < x \le L.
\end{aligned}
\tag{9}
$$

The initial conditions are

$$
\begin{aligned}
&u_x(x,y,t)\,|_{t=0} = 0, \quad u_y(x,y,t)\,|_{t=0} = 0, \quad u_z(x,y,t)\,|_{t=0} = 0,\\
&w_x(x,y,t)\,|_{t=0} = 0, \quad w_y(x,y,t)\,|_{t=0} = 0, \quad w_z(x,y,t)\,|_{t=0} = 0,\\
&\frac{\partial u_x}{\partial t}(x,y,t)\,|_{t=0} = 0,\ \ \frac{\partial u_y}{\partial t}(x,y,t)\,|_{t=0} = 0\ \ \text{and}\ \ \frac{\partial u_z}{\partial t}(x,y,t)\,|_{t=0} = 0.
\end{aligned}
\tag{10}
$$

For the parameters of a three-dimensional icosahedral Al–Pd–Mn quasicrystal, the measured mass density $\rho = 5.100 \times 10^{-3}\,\mathrm{g{\cdot}mm^{-3}}$ is used and elastic moduli are taken as L=0.75, M=0.65($10^{12}\,\mathrm{dyn/cm^2}$), K_1=0.00072, $K_2 = -0.00037(10^{12}\,\mathrm{dyn/cm^2})$[13] and $\Gamma_w = 1/\kappa = 4.8 \times 10^{-7}\,\mathrm{cm^3 \cdot \mu s/g}$.[14] The coupling constant R has not been measured so far. In the computation, we take $R/M = 0.001$ as a coupling case corresponding to the quasicrystal. In the following section, we will take $H = 20\,\mathrm{mm}$, $L = 10\,\mathrm{mm}$ and the crack initial length $a = 2.4\,\mathrm{mm}$.

At present, the analytic solutions for the initial-boundary value problems represented by Eqs.(7), (9) and (8) are not available due to their complexity, so the numerical method has to be used to solve these equations. Here we extend the finite difference method in the scheme presented by Shmuely and Alterman,[15] used to analyse crack problems in conventional engineering materials, to the case of quasicrystalline materials.

3. The finite difference scheme

A grid is imposed on the upper right of the specimen as shown in Fig.2. For convenience, the values of mesh size h are taken to be identical with each other in both x and y directions. The grid is extended by half a step due to adding four special grid lines $x = -h/2$, $x = L + h/2$, $y = -h/2$, and $y = H + h/2$, which form the grid boundaries. Using difference formulations, numerical results of stress, phason displacement and stress intensity factors are obtained.

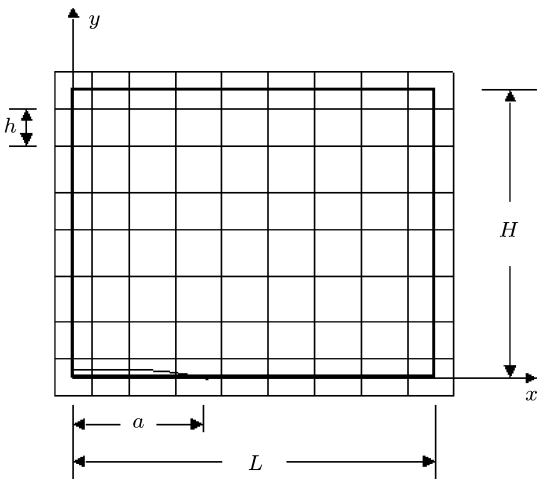


Fig.2. Grid mesh finite difference.

4. Dynamic response of the icosahedral Al–Pd–Mn quasicrystal with a Griffith crack to impact loading

Variations of phason displacement components w_x and w_y of a three-dimensional icosahedral Al–Pd–Mn quasicrystal with time are shown in Fig.3. As seen from Fig.3, when $t \leq T_0$ the displacements of phonon field and phason field are both equal to zero, because the wave from the boundary has not arrived at the crack tip. In the figure $t = T_0 = 0.9741\,\mu$s represents the time when the wave propagates from the external boundary to the crack surface, so the speed of the wave propagation is $v = H/T_0 = 20.5321\,$km/s, which is just equal to the longitudinal wave speed $c_1 = \sqrt{(L+2M)/\rho}$. When the wave arrives at the crack tip at $t = T_0$, the displacements descend with the time until $3.3\,\mu$s then approach a stable state. We also notice that both displacements w_x and w_y have a similar trend, however, the value of w_x is bigger than that of w_y.

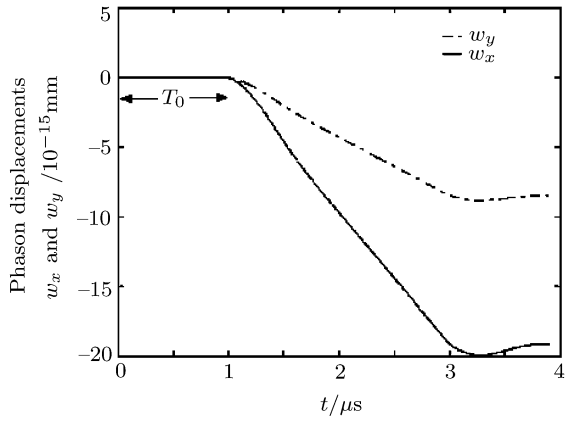


Fig.3. Phason displacements w_x and w_y for the icosahedral Al–Pd–Mn quasicrystal.

Variations of stress intensity factors of phonon field and phason field with time are shown in Figs.4 and 5 respectively. The normalized dynamic stress intensity factor for phonon field, $K_I^{\parallel}(t)/\sqrt{\pi a_0}p$, is used in Fig.4, in which the dynamic stress intensity factor $K_I^{\parallel}(t)$ is defined as

$$K_I^{\parallel}(t) = \lim_{x \to a_0^+} \sqrt{\pi(x-a_0)}\sigma_{yy}(x,0,t). \qquad (11)$$

The phonon field is in the physical space or the parallel space, which is labelled by the superscript '$\parallel$'. The normalized dynamic stress intensity factor for phason field, $K_I^{\perp}(t)/\sqrt{\pi a_0}p$, is used in Fig.5, in which the dynamic stress intensity factor $K_I^{\perp}(t)$ is defined as

$$K_I^{\perp}(t) = \lim_{x \to a_0^+} \sqrt{\pi(x-a_0)}H_{yy}(x,0,t). \qquad (12)$$

The phason field is in the complement space or the vertical space, which is labelled by the superscript '$\perp$'.

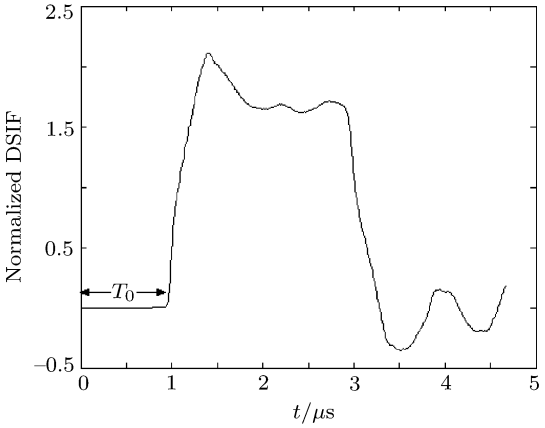


Fig.4. Variation of normalized dynamic phonon field stress intensity factor (S.I.F) with time.

It can be observed that the stress intensity factors of phonon field and phason field both present wave propagation, although the phason field satisfies the diffusion equation. Because the influence of the phonon field on the phason field is big, i.e. the wave propagation is predominant in the elastohydrodynamics of quasicrystals. An interesting point is that the stress intensity factors of phonon field and phason field are opposite in the tendency of variation, that is, the stress intensity factor of phonon increases sharply at about $1\,\mu$s while the stress intensity factor of phason decreases abruptly at about $1\,\mu$s. The stress intensity factor of phason is negative in Fig.5, which is interesting. We believe that the phason field presents

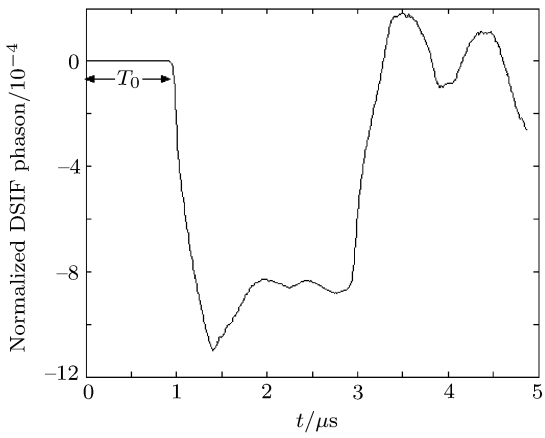


Fig.5. Variation of normalized dynamic phason field stress intensity factor (S.I.F) with time.

a kind of the compression wave, which leads the surface of the crack to have a closing tendency. From the two figures, the order of magnitude of phason field seems to be much smaller than that of phonon field, for which one reason lies in the choice of boundary conditions in the present formalism, where the boundary conditions corresponding to phason field are taken to be zero (because measured data are unavailable so far, the simplest way of treating them is to assume the stress boundary values of phason to be zero). Otherwise if we adopt nonzero boundary conditions for the phason field, the computation results will show the order of magnitude of phason variables to be greater.

In order to reveal the features of the wave propagating in the quasicrystals, we plot the results of six stress components of the phonon field and phason field in Fig.6, with stress being in units of $\mathrm{g}\cdot\mathrm{mm/ms}^2$.

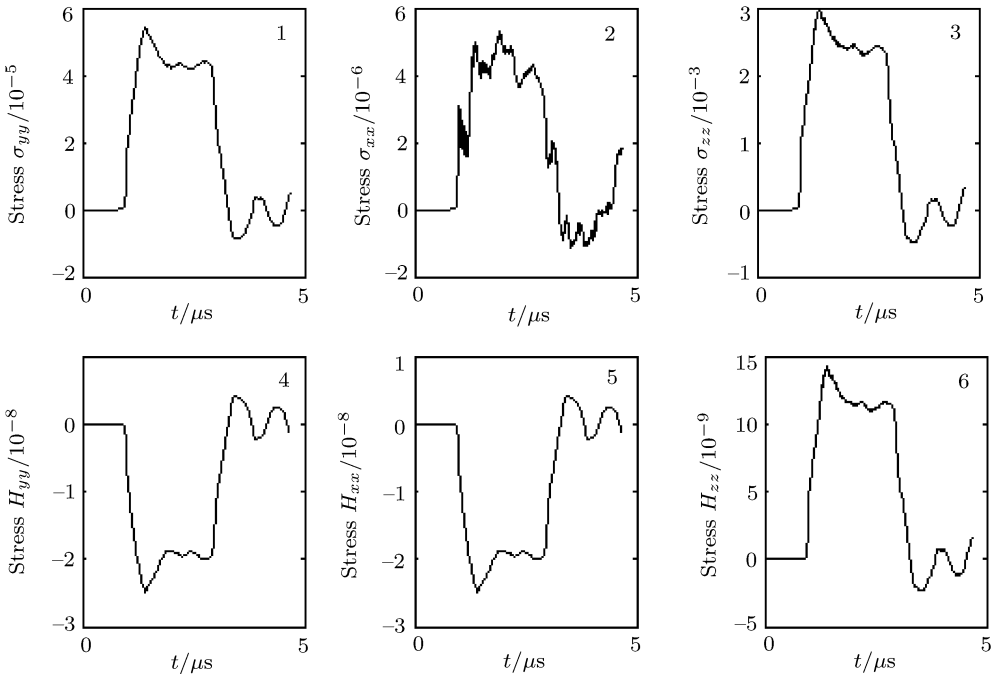


Fig.6. Variations of six stress components of the icosahedral Al–Pd–Mn quasicrystal with time.

To indicate the dynamic behaviours of phason field under the nonzero boundary conditions, a configuration the same as that shown in Fig.1 is reconsidered. Its boundary conditions can be expressed as follows:

$$
\begin{aligned}
&u_x = 0,\ \sigma_{xy} = 0,\ \sigma_{xz} = 0,\ w_x = 0,\ H_{xy} = 0,\\
&\text{and}\ \ H_{xz} = 0\ \ \text{on}\ \ \ x = 0\ \ \ \text{for}\ \ 0 \le y \le H;\\
&\sigma_{xx} = 0,\ \ \sigma_{xy} = 0,\ \ \sigma_{xz} = 0,\ \ H_{xx} = 0,\ \ H_{xy} = 0,\\
&\text{and}\ \ H_{xz} = 0\ \ \text{on}\ \ \ x = L\ \ \ \text{for}\ \ \ 0 \le y \le H;\\
&\sigma_{yy} = 0,\ \ \sigma_{yx} = 0,\ \ \sigma_{yz} = 0,\ \ H_{yy} = p(t),\ \ H_{yx} = 0,\\
&\text{and}\ \ H_{yz} = 0\ \ \text{on}\ \ \ y = H\ \ \ \text{for}\ \ 0 \le x \le L;\\
&\sigma_{yy} = 0,\ \ \sigma_{yx} = 0,\ \ \sigma_{yz} = 0,\ \ H_{yy} = 0,\ \ H_{yx} = 0,\\
&\text{and}\ \ \ H_{yz} = 0\ \ \ \text{on}\ \ y = 0\ \ \ \text{for}\ \ 0 \le x \le a;\\
&u_y = 0,\ \ \ \sigma_{yx} = 0,\ \ \ \sigma_{yz} = 0,\ \ \ w_y = 0,\ \ \ H_{yx} = 0,\\
&\text{and}\ \ H_{yz} = 0\ \ \text{on}\ \ y = 0\ \ \text{for}\ \ a < x \le L. \qquad (13)
\end{aligned}
$$

A comparison between Fig.4 and Fig.7 shows that the stress intensity factor (in Fig.4) is positive under the boundary conditions (9), however, the propagating wave is negative under the boundary conditions (13), i.e. as the external loading varies from the phonon field to the phason field, the stress wave changes from extending to compressing. The order of

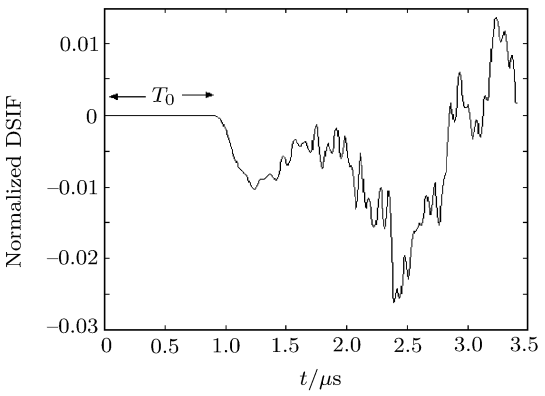


Fig.7. Variation of normalized dynamic phonon field stress intensity factor (S.I.F) with time.

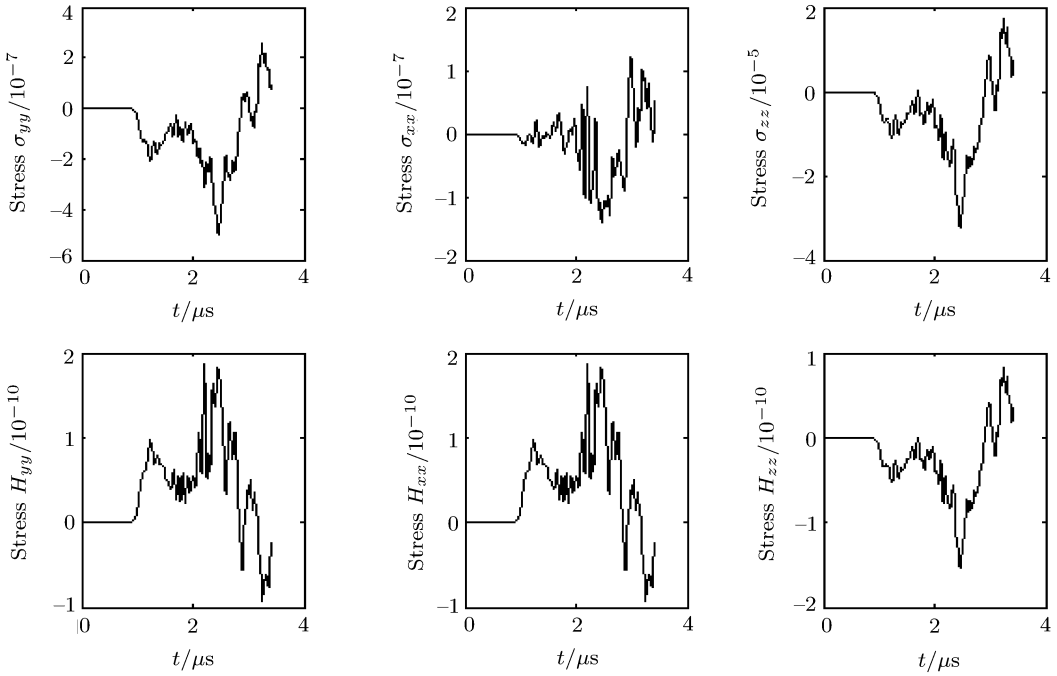


Fig.8. Variations of six stress components of the icosahedral Al–Pd–Mn quasicrystal with time.

magnitude of phason field increases under the condition of the external loading. Similarly, the stresses also have the same features when we change the boundary conditions, as those shown in Figs.6 and 8, with stress being in units of $\mathrm{g}\cdot\mathrm{mm/ms}^2$.

5. Conclusion and discussion

According to the elasto-hydrodynamics model, the phason degree is considered as a diffusion motion, so its influence on phonon wave propagation is very small. But the influence of phason on the dynamic response of the icosahedral Al–Pd–Mn quasicrystal with a Griffith crack to impact loading cannot be neglected due to the phonon–phason coupling effect.

In Ref.[16] the crack propagation in two-dimensional decagonal quasicrystals was discussed by using the molecular dynamic simulation, which put forward the conception of 'phason wall'. This viewpoint accords with the fact that phason field yields a compressed wave as indicated in our paper. It should be pointed out that Ref.[16] and our paper demonstrate this conception from microscopic and macroscopic aspects, respectively.

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