0.1 Crack propagation in quasicrystals

Christoph Rudhart\textsuperscript{a}, Peter Gumbsch\textsuperscript{b,c}, and Hans-Rainer Trebin\textsuperscript{a}

\textsuperscript{a} Institut für Theoretische und Angewandte Physik, Universität Stuttgart
D-70550 Stuttgart, Germany

\textsuperscript{b} Institut für Zuverlässigkeit von Bauteilen und Systemen, Universität Karlsruhe
D-76131 Karlsruhe, Germany

\textsuperscript{c} Fraunhofer Institut für Werkstoffmechanik
D-79194 Freiburg, Germany

0.1.1 Introduction

When a solid is ruptured, mechanical energy of a large volume is concentrated to an atomically
sharp crack tip to break chemical bonds. Fracture, hence, is a phenomenon that spans different
lengths scales. Its study requires a variety of physics tools ranging from quantum mechanics
and classical molecular dynamics to continuum mechanics.

Linear elastic fracture mechanics is treating cracks as free internal planar surfaces of an
elastic continuum. This results in a singularity of the stress field that decays as the inverse
square root of the distance $R$ from the crack tip [1]:

$$
\sigma_{ij} = \sum_{\alpha=1}^{3} K_{\alpha} \frac{1}{\sqrt{2\pi R}} f_{ij}^{\alpha} (\theta),
$$

(1)

where $f_{ij}^{\alpha}$ are functions of the angle $\theta$ between $R$ and the crack plane. The strength of the
singularity is characterized by the stress intensity factors $K_{\alpha}$ for mode $\alpha$ loading (I = opening,
II = in-plane shear, III = out-of-plane shear). Although the geometry of the specimen and its
macroscopic dimension determine the stress concentration at the crack tip, the occurrence of
the square root singularity is independent from the particular loading conditions. The linear
elastic continuum description allows to calculate the values of the stress field but it does not
answer the question, under which conditions a crack will propagate. An explicit fracture
criterion to predict crack propagation is the Griffith criterion. It can be formulated as a balance
of the crack driving force, the energy release rate $G$, and the surface energy $2\gamma$ of the two
freshly exposed fracture surfaces: $G = 2\gamma$. For pure mode I loading $G$ is related to the
stress intensity factor by $G = K_{I}^2 / E'$, where $E'$ is an appropriate elastic modulus [1]. This
criterion implies the assumption of thermodynamic equilibrium for the crack tip. Since crack
propagation is clearly a non-equilibrium phenomenon, the Griffith criterion constitutes only
a necessary condition for crack propagation. It does not explain in which direction the crack
will propagate [2].

The continuum description poses two major problems. First, the stress singularity leads to
infinite stresses at the crack tip. Thus in its vicinity the linear elastic continuum description
loses validity. Second, the atomistic character of the material is not taken into account. Al-
though the anisotropic linear elastic continuum analysis of a sharp crack tip [1] considers the
crystallographic orientation of the crack system via appropriate elastic constants it is not able
to describe phenomena that arise from the detailed geometry of the atomic bonds. An exam-
ple how the atomistic structure influences crack propagation is the so-called lattice trapping
effect [3]. It causes the crack to be stable and not to advance until loads are applied that are
somewhat larger than the Griffith value. The lattice trapping can be viewed as the equivalent
of the Peierls barrier, which impedes the motion of a dislocation. The magnitude of the trap-
ping depends on the detailed arrangement of the bonds at the crack tip. Thus the barrier for
the crack to advance can vary significantly for different orientations of the crack front on the
same fracture plane [2]. Indeed a pronounced anisotropy is observed experimentally for both
single crystalline metals [4] and semi-conductors [5, 6].

Materials are classified as brittle if they shatter like glass and ductile if they are deformable.
Whereas perfectly brittle materials fail without significant plasticity, ductile failure is associ-
ated with large plastic deformations. Whether a crystalline material is intrinsically brittle or
ductile depends on its ability to emit dislocations from the crack tip. Once a dislocation has
nucleated, its stress field can shield the forces acting on the crack tip and prevent the crack
from moving. In addition, the driving force on the crack tip is lowered because the dislocation
can blunt the crack tip. Thus cleavage and dislocation emission can be seen as competing
processes for the failure of crystals. A simple criterion to decide whether a crystal is brittle
or ductile was proposed by Rice and Thomson [7]. It is based on the calculation of the forces
that act on a fully formed dislocation in the presence of a sharp crack. This force turns out
to be attractive for small distances \( r \) but becomes repulsive for large values of \( r \). The crack
is considered as stable against emission of a blunting dislocation when the equilibrium dis-
tance \( r_0 \) is small, compared to a characteristic length, the so-called core cut-off radius of the
blunting dislocation.

More sophisticated methods that consider the atomic structure of the blunting dislocation
use the Peierls concept in the analysis of dislocation formation at the crack tip [8, 9]. The
resistance of the crack to dislocation nucleation is then approximately characterized by the
so-called unstable stacking fault energy \( \gamma_{ua} \). It represents the energy barrier that has to be
overcome for a dislocation to nucleate from the crack tip.

Ductile failure is favored also, if other dislocation sources near the crack tip allow nucle-
ation of new dislocations. This usually occurs at much lower stresses than predicted by the
Peierls model. In either case, once nucleated the dislocation has to be able to move away from
the crack tip to build a reasonably sized plastic zone. The latter requires sufficient dislocation
mobility, which is the reason why the brittle or ductile response also depends on temperature
and loading rate [10]. While for crystals there exist different models for the brittle-to-ductile
transition, it is less well understood in amorphous or quasicrystalline materials [11]. Essen-
tially, the concepts are all based on the periodicity of the underlying structures and do not
directly apply to quasicrystals. In the current work we study the influence of dislocation nu-
cleation on crack propagation of model quasicrystals.

The behavior of single quasicrystals under mechanical loads has been the subject of nu-
merous studies in the last years (for reviews, see [12] and [13]). The main results are a pro-
nounced brittle-to-ductile transition (BDT) at about 80% of the melting temperature \( T_m \) and
a good deformability up to 20% without hardening above the BDT. These properties are at-
tributed to the peculiar structure of quasicrystals. On one hand, quasicrystals are cluster-based
structures. The clusters act as obstacles to moving dislocations which are responsible for the
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As a result moving dislocations are always followed by planar defects, so-called phason walls [14]. The phason walls and the clusters are believed to play the main parts in the process of plastic deformation.

In contrast, experiments on crack propagation in single quasicrystals are scarce. Most are indentation tests where the fracture toughness is estimated from the geometry of the indentations, the applied external force, and the length of the microcracks emitted from the indenter corners [15]. The values for the fracture toughnesses at room temperature are about 1 MPam$^{1/2}$ [15, 16] which is close to those for brittle ceramics or silicon [2]. The cracks in the vicinity of microhardness indentations are observed to propagate predominantly along well-defined crystallographic planes [15]. Investigations of cleavage surfaces by scanning tunneling microscopy clearly show that the structure of fracture surfaces [17] is influenced by clusters. However, the atomistic scale is not accessible to experiments if the dynamics of the fracture process is concerned.

Molecular dynamics is used extensively to study the fracture process in both periodic crystals and amorphous solids. Up to now simulations and most of the experiments have been performed at low temperatures [18, 19, 20, 21], where quasicrystals fail by brittle fracture. Fracture at higher temperatures and the BDT have not been studied yet.

Here we apply molecular dynamics simulations to study the dynamic crack propagation in a wide range of temperatures. We use simple two-dimensional models which display the main characteristics of quasicrystals. Thus our simulations provide an indication of the characteristic features and the elementary processes that dominate the fracture process in real quasicrystals.

0.1.2 Models and method

To study crack propagation by molecular dynamics [22] one has to choose a structure model and a suitable model for the atomic interaction. Since the atomistic model can only answer questions that are within its validity, it is crucial to take great care in selecting a suitable interaction. For metals and covalent systems there exist a wide range of semi-empirical materialspecific potentials that mimic real materials. For most quasicrystals realistic interactions and structure models are not available at the moment. We therefore choose a generic pair potential...
to model the atomic interactions and do not make the attempt to mimic one particular material.

To evade the analysis of a three dimensional crack front the analysis is restricted to simple two-dimensional models. We use two different structures, a perfectly ordered and a randomized model quasicrystal. Both models are obtained by decoration of quasiperiodic tilings. In the following the expression tiling is used as a synonym for the atomic representation. The Mikulla-Roth tiling (MRT) [23] is obtained from the decagonal Tübingen triangle tiling [24] by placing large (A) atoms on the vertices and small (B) atoms on the circumcenters of the large triangles. The MRT shares central properties with structure models for real quasicrystals, namely a quasiperiodic plane structure and a hierarchical structure of decagonal clusters. The smallest clusters are given by concentric rings of ten small and ten large atoms (Fig. 1), and can be considered as two-dimensional versions of Mackay clusters which are significant for real quasicrystals. The clusters themselves are arranged on families of parallel planes (Fig. 2). The planes occur with two different distances, according to a Fibonacci sequence. Due to the decagonal symmetry of the system, equivalent families of lines result from rotations by 36°.

The random tiling model is constructed from a perfectly ordered MRT by increasing the phason degree of disorder through random phason flips [25]. The symmetry of the resulting random tiling is still decagonal as for the MRT but the frequencies of the atomic surroundings are different. The tenfold clusters of the MRT are mostly destroyed.

Figure 2: The binary model quasicrystals: MRT (top) and random tiling (bottom). Left: Bond representation obtained by connecting nearest neighbors of different types. Right: Atomic representation where the two species of atoms are represented as discs. Planes with low surface energy are indicated by light lines.
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Fig. 2 shows the two model quasicrystals in two different representations. In the atomic representation the two species of atoms are represented as discs. The bond representation is obtained by connecting nearest neighbors of different type. Defects in quasicrystals are always associated with the occurrence of forbidden local surroundings. Thus the bond representation is particularly suitable to display dislocations and phason walls.

Both model quasicrystals, the MRT and the random tiling system are decagonal binary tilings (BT). BT are mixtures of two species of particles where the bond length fulfill the requirement that five particles of type A surround one B particle and ten B particles surround one A particle. The atomic interactions are modeled by Lennard-Jones (LJ) potentials [26], originally derived for the van der Waals-type interaction of inert gases. For the binary systems we have to specify potentials for the AA, BB, and AB interactions, respectively (see Fig. 3). The bond lengths are chosen to be the geometrical ones. The depths of the LJ potentials are $\epsilon_0$ for AA and BB bonds and $2\epsilon_0$ for AB bonds. With this choice of parameters for the LJ potentials the highest coordinated decagonal clusters become the tightest bound structural units of the quasicrystal. The unit of length $r_0$ is the same for all three interactions and corresponds to the length of one AB bond in the structure. All masses are set to unity and the time is measured in units of $t_0 = r_0\sqrt{m/\epsilon_0}$.

As mentioned above, the stress field of the crack is characterized by a weak $1/\sqrt{R}$ singularity. For molecular dynamic studies, where only a finite number of atoms can be treated, the long range character of the stress field has to be considered via appropriate boundary conditions. One possibility is to choose a large sample where the border atoms of the sample are held fixed and the atoms are displaced according to the linear elastic solution of a semi-infinite stable crack. The crack tip region is then relaxed to find the minimum energy configuration. Subsequently the system is driven into a mechanical instability by gradually increasing the strain on the borders until the crack propagates. These boundary conditions are particularly appropriate for simulations where material-specific interactions allow to calculate

![Figure 3: Lennard–Jones–Potentials for the three interactions. The depth of the potentials are $\epsilon_0$ for AA and BB bonds and $2\epsilon_0$ for AB bonds.](image-url)
the load at which the instability of the mechanical system occurs. Due to the long range character of the stress field and the need to specify the location of the crack tip these boundary conditions are not suitable, however, to study dynamic crack propagation.

A different method which is applied here is to choose boundary conditions so that the system can reach a steady state. For this purpose we use a strip geometry to model crack propagation with constant energy release rate [27]. Our samples consist of about 330,000 atoms in a strip of width 275 $r_0$ which corresponds to an aspect ratio of 3.5. The strip is homogeneously strained perpendicular to its long axis and an atomically sharp crack is inserted from one short side to one third of the strip length. All atoms in the outermost boundary layer of width 3$r_0$ remain fixed during the simulation. Subsequently the sample is relaxed to obtain the displacement field of the stable crack at zero temperature. The strip is chosen long enough to ensure that the crack surfaces at the pre-cracked side of the strip are fully relaxed. The opposite boundary in front of the crack is homogeneously strained. The crack advance can be viewed as replacing a strip of material that is homogeneously strained by a strip with two fully relaxed surfaces. The energy difference is of course independent of the crack tip position and the crack thus propagates with a constant energy release rate and at a constant driving force irrespective of its position in the strip.

To stabilize the crack at finite temperatures we scale the zero temperature crack field considering the thermal expansion of the system. The displacement field is obtained by averaging over the atomic positions for several thousand time steps to eliminate the thermal motion of the atoms. Afterwards the crack is loaded by adding a fraction of the averaged displacement field to the stable crack. The system is initially strained to the Griffith load where the energy release rate per unit length of crack extension $G$ is equal to the surface energy of the two crack surfaces $2\gamma$. It should be noted that the Griffith criterion provides only a rough approximation.
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Figure 5: Crack propagation mechanism in the MRT. (a) The crack propagates on the initial fracture plane. (b) It has emitted a dislocation that is followed by a phason wall. (c) The quasicrystal has opened up along the phason wall.

of the critical load. Due to the quasiperiodicity of the structure, this critical value is not unique but depends on the crack tip position [28]. The overloads are given by $\Delta K^*$ in the following, which is the fraction of the displacement field that is added to the stable crack.

According to the Griffith criterion, planes with low surface energy are potential fracture planes. To identify those planes we relax a specimen and split it in two regions. Subsequently, the two parts are shifted rigidly by a distance of $10 r_0$ perpendicular to the cutting plane. The surface energy is then calculated from the difference of the artificially cleaved and the undisturbed specimen.
Figure 6: Disregistry energy along a glide plane. The energy for the relaxed phason wall of the first minimum is about 14% of the surface energy.

For simple crystal structures like the face centered cubic structure of the noble metals the surface energy only depends on the crystallographic orientation of the surface. In quasicrystals, however, it even varies for crystallographically equivalent but structurally distinct surfaces. Fig. 4 shows the surface energy for crystallographically equivalent surfaces as a function of the position of the cutting plane. In the MRT we find a pronounced plane structure of low and high surface energies. The planes of lowest surface energy occur with two separations, arranged in a Fibonacci sequence. These correspond to the planes between the large separation of the parallel lines connecting the clusters and are given by the light lines in Fig. 2. The random tiling shows no such distinct plane structure. For the random tiling the difference between the planes of lowest and highest energy is only about $0.2 \epsilon_0/r_0$ while for the MRT it is about $0.5 \epsilon_0/r_0$. We select the surfaces of lowest energy as initial fracture planes for the simulations in the MRT.

0.1.3 Low temperature crack propagation

In the low temperature regime of below $0.10 T_m$, crack propagation in both model systems the perfectly ordered and randomized system is studied in dependence on the load. Acoustic waves emanating from the crack tip are absorbed by ramping up a viscous damping from a small finite value at the fracture plane to a maximum value at the boundary [27].

For small loads up to $\Delta K^* = 0.2$ the crack propagates only a few atomic distances $r_0$ and then stops for both systems. The minimal velocity for brittle crack propagation is about 15% of the shear wave velocity $v_s$. The cracks are stopped by obstacles like incomplete tenfold clusters that are contained in both systems.
For loads in the range of $\Delta K^* = 0.30$ to $0.50$ the crack velocity increases with the applied load just as in periodic crystals. However, the mode of propagation in the MRT differs significantly from that in periodic systems [18, 19, 20, 21]. The crack propagates on the initial fracture plane until it hits an obstacle. There a dislocation nucleates along a plane that is inclined by $36^\circ$ (Fig. 5a). The dislocation does not get farther away from the crack tip than
Figure 8: Snapshot at $\Delta K^* = 1.10$ and $T = 10\% \ T_m$. The branches follow the easy planes that are inclined to the fracture plane by $36^\circ$.

$5r_0$ before it is blocked by another obstacle (Fig. 5b). This is in agreement with simulations of dislocation mobility [14] which show that complete or incomplete clusters act as obstacles for moving dislocations. As mentioned above, the stress field of the dislocation generally is expected to shield the crack from the applied load which results in an increase of fracture toughness. Here, however, the crack follows the dislocation as can be seen in Fig. 5 c). This can be explained by the aperiodic structure of quasicrystals.

Quasiperiodic structures can be obtained as cuts of an irrationally oriented $n$-dimensional hyperplane (physical space) through a $d$-dimensional periodic crystal [29], where $d > n$. Due to the periodicity of the hyper-crystal, the $d$-dimensional Burgers vectors carry a $n$-dimensional component $b^\parallel$ in physical space and a $(d - n)$-dimensional component $b^\perp$ in the complementary orthogonal space. A moving dislocation in a quasicrystal leaves in its wake a plane defect that separates two areas with a phase difference $b^\perp$. This defect which gives rise to differences in the atomic environments compared to the perfect quasicrystal is called a phason wall [30].

Fig. 6 shows the disregistry energy [30], which is the potential energy necessary to shift one half of a quasicrystal rigidly over the other along a glide plane. For periodic crystals this energy is called $\gamma$-surface [31] and is a periodic, approximately sinusoidal curve with zero fault energy at multiples of the lattice vectors. For our model quasicrystal the disregistry energy is quasiperiodic with two classes of local minima. Those of the first class are very deep with values of the order of $10^{-4}$ and represent the primary Burgers vectors of the model. The disregistry energy for the minima of the second class are of the order of 1. In contrast to periodic crystals, the disregistry energy does not vanish but remains finite for any arbitrary choice of the displacement.

The Phason wall behind a dislocation emitted by the crack tip corresponds to the first minimum of the second class. The disregistry energy is about $50\%$ of the surface energy $\gamma$ and is reduced by elastic relaxation to about $14\%$ of $\gamma$. Thus, along this wall the structure is weakened and the cohesive energy diminished, with the consequence that the material is preferably opening in this plane. The resulting fracture surface shows characteristic deviations of $36^\circ$ to the initial fracture plane (see Fig. 7).
To confirm the mechanism we construct artificially a phason wall and simulate crack propagation along it. The wall is introduced by cutting the sample into halves along the fracture plane. Then the upper part is shifted rigidly for the length of the Burgers vector $b$ in the direction parallel to the fracture plane. This yields a phason wall comparable to the one behind a dislocation with Burgers vector $b = 1.1$ which corresponds exactly to the phason wall we had observed in the fracture simulations. Dislocations with the same Burgers vector were also observed in shear simulations [32]. Subsequently we stabilize a crack on the phason wall according to the procedure prescribed in Section 0.1.2. As a result the crack propagates without changing direction as can be seen in Fig. 7.

The random tiling displays no plane structure (Fig. 2). Thus the dislocation nucleation process is suppressed and the crack propagates by the breaking of individual bonds. In contrast to the simulations in the MRT we do not observe the zig-zag shape of the fracture surface. Crack configurations from simulations at $0.10 T_m$ for the two systems are shown in Fig. 7. The obstacles that cause the crack in the MRT to deviate from the initial fracture plane, incomplete stable clusters are also avoided rather than cut by the crack in the random tiling.

At loads above $\Delta K^* = 0.5$ the crack becomes unstable and branches. A typical configuration for the crack branching at $0.10 T_m$ and a load of $\Delta K^* = 1.00$ is shown in Fig. 8. The branches form an angle of $\theta = 72^\circ$ and correspond again to the easy planes which are located at every $36^\circ$ inclination from the fracture plane. The determination of a single crack tip position is obviously impossible. The crack velocity of the branches can roughly be estimated to lie in the range of $0.4 - 0.5 v_c$.

Although the mechanisms of crack propagation are different the dependence of the crack tip velocity on the applied load is essentially the same for the two systems (Fig. 9). Simu-
lations of crack propagation in periodic crystals show that the crack tip speed increases with the applied load to a maximum value of about $40\%v_s$. Further increase of the load does not significantly change the terminal velocity. This is explained by the non-linearity of the atomic interaction [16]. In our simulations the velocity increases with the load until the crack bifurcates. We do not observe a plateau of constant velocity. For the propagation along the phason wall, the occurrence of the instability is shifted to higher loads of $\Delta K^* = 0.80$. For crack propagation along the phason wall we do observe an almost constant crack tip speed for loads between $\Delta K^* = 0.50$ and $\Delta K^* = 0.70$.

### 0.1.4 Finite temperature crack propagation

In the low temperature regime the Griffith criterion was used to estimate the critical load for a stable crack. At zero temperature the critical load can be calculated by straining the sample until the change in elastic energy equals the potential energy necessary to cut the sample (artificially) into parts. For low temperatures the critical load can be approximated from the zero temperature elastic constants that are easily accessible by molecular dynamics. For finite temperature this procedure is no longer possible since all transformations are connected with changes in the free energy of the system. Thus to apply the Griffith criterion at finite temperature the free energy of both transformations must be calculated [33].

As mentioned above the Griffith criterion, although referred to as a criterion, provides only a necessary condition for crack propagation but does not explain how the crack propagates. In addition it does not consider the possibility of plastic deformation in the vicinity of the crack tip. In our simulations we observe that for temperatures above $30\% T_m$ the crack does not remain atomically sharp but blunts spontaneously. Thus, in this temperatures regime the Griffith criterion cannot predict whether the crack will propagate or not. In addition it is not possible to average over a sufficiently large number of time steps to obtain a stable initial condition for a sharp crack.

**Figure 10:** Sketch of the strip geometry for the simulations with temperature gradient. The sample is scaled to balance the thermal expansion of the sample.
To overcome this problem and to nevertheless study brittle crack propagation at higher temperatures we introduce a new simulation geometry which mimics an experimental setup which is used to study the BDT [34, 35]. In these experiments a crack is driven up a temperature gradient from a cold region where it propagates by brittle cleavage to a high temperature region, where it suddenly arrests. By measuring the temperature gradient along the sample, the brittle to ductile transition temperature for a given loading rate can be determined from the position of the crack arrest.

We use a very long strip of the same width as in the low temperature simulations but with an aspect ratio of 10. A linear temperature gradient is applied along the strip and the crack is introduced on the low temperature side where a sharp tip can be stabilized. The crack is then driven into a region of elevated temperature (Fig. 10) by loading the sample as described in Section 0.1.2. A local temperature control scheme [36, 27] was used to establish the temperature gradient. Corresponding to the applied temperature gradient, the system is expanded to balance the thermal expansion, which results in a telescope shape of the specimen (Fig. 10). The crack is stabilized in a region with \( T = 0.3 T_m \) and the temperature is increased to \( 0.8 T_m \) on a length of \( 1500 \ v \). Acoustic waves emanating from the crack tip are absorbed by ramping up a viscous damping from a small finite value at the fracture plane to a maximum value at the outer boundary [27].

Crack propagation in the strip geometry with temperature gradient is studied exclusively in the MRT. Corresponding to the temperature gradient, the tip position can be directly translated into a temperature at the position of the crack tip (Fig. 10).
Figure 12: Crack before (left) and after (right) blunting. The glide plane of the dislocation is inclined by $72^\circ$ to the initial fracture plane. The Burgers vector of the blunting dislocation is visualized by the Burgers circuit.

For small overloads $\Delta K^* \leq 0.30$ and shallow temperature gradients the crack travels at almost constant velocity until a dislocation nucleates along a plane that is inclined by $72^\circ$ to the initial fracture plane (see Fig. 12). The crack then stops in the medium temperature regime between $30 - 70\% T_m$ by spontaneous blunting of the crack tip. Just like in the low temperature regime, the dislocation does not get farther away from the crack tip than $5r_0$ before it is blocked by an obstacle. In contrast to the dislocation-emission-phason-wall mechanism on the $36^\circ$ plane in the low temperature regime, the blunting dislocation on the $72^\circ$ plane of elevated temperature is able to shield the crack from the applied load, and the crack does not follow the path of the dislocation. In the case of the blunting dislocation the opening stress on the phason wall is apparently too small on the highly inclined glide plane.

For loads above $\Delta K^* = 0.40$ the blunting dislocation is no longer able to shield the crack. We still observe the nucleation of blunting dislocations but in contrast to the behavior for smaller overloads a new crack is formed from the dislocation core. As a result the crack is driven into the high temperature regime.

At temperatures above $70\%$ of $T_m$ the velocity of the crack drops considerably (see Fig. 11) but the crack does not stop. The decrease in velocity corresponds to a change in propagation mechanism. The crack does no longer propagate with an atomically sharp crack tip but rather extends by nucleation, growth and coalescence of microvoids (Fig. 13). A similar behaviour is observed in molecular dynamics simulations of fracture in model non-crystalline solids [11].
Here the plastic deformation is observed to be localized to so-called shear transformation zones [37]. In our simulations we observe an increase of breaking bonds in the vicinity of the crack tip but we do not observe any dislocations. Fig. 13, for example, shows such a gradual, dislocation-free crack extension. Obviously the crack does not follow a favored fracture plane. Thus for high temperatures our model quasicrystal shows a glass-like behaviour.
0.1.5 Conclusion

In this section crack propagation of mode-I cracks was studied in two-dimensional decagonal model quasicrystals by molecular dynamics simulations. In particular, the dependence on temperature, applied load and underlying structure has been investigated.

For low temperatures up to 30% of the melting temperature $T_m$, our model quasicrystals fail by brittle fracture. Just like in periodic crystals the crack tip velocity increases with the applied load until the crack becomes unstable and branches. In this low temperature regime the crack tip velocities are about $20\%-50\%$ of the shear wave velocity $v_s$. Although the dynamics of the crack tip is similar to that in periodic crystals, the mode of propagation differs significantly. We observe dislocation nucleation from the crack tip on a glide plane that is inclined by $36^\circ$ to the fracture plane. A dislocation in a quasicrystal is always followed by a phason wall. The cohesive strength of the quasicrystal is reduced along this wall, with the consequence that the material is opening up along this defect. Thus, dislocation nucleation does not yield in an increase of fracture toughness as in periodic crystals and the model quasicrystals fail by dislocation-mediated brittle fracture.

For temperatures above 30% of $T_m$ the crack does not remain atomically sharp but blunts spontaneously. To deal with this fact and to nevertheless study a sharp crack a new type of boundary condition with a linear temperature gradient is established along a strip. From the low temperature regime, where a sharp tip can be stabilized, the crack is driven into a region of elevated temperature.

In the range of 70% - 80% $T_m$ the failure mode of the quasicrystal changes and the crack advances by void formation and coalescence. In summary, at low temperatures the crack propagates along crystallographic planes just like in periodic crystals, whereas a glass-like ductile growth mode is dominant at high temperatures.

Acknowledgments

Financial support from the Deutsche Forschungsgemeinschaft under Project Tr 154/13 is greatly acknowledged.

Bibliography

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