Crack Propagation in Icosahedral Model Quasicrystals

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Summary. Propagation of mode-I cracks in a three-dimensional model quasicrystal is studied by molecular dynamics simulations. The samples are endowed with an atomically sharp crack and subsequently loaded by linear scaling of the displacement field. The response of the system is then monitored during the simulation. In particular, the crack surface morphology is investigated in dependence of the orientation of the fracture plane. For this purpose, fracture surfaces perpendicular to two- and fivefold axes are compared. For both directions, brittle fracture with rough fracture surfaces is observed.

1 Introduction

Quasicrystals are intermetallic alloys whose diffraction patterns display sharp Bragg peaks with non-crystallographic point symmetries. Therefore their mass density is quasiperiodic rather than periodic. Most concepts used to predict the response of a material to an applied load are (at least on an atomic scale) based on the periodicity of the underlying structures, and thus do not apply to quasicrystals.

Although it is possible to grow single quasicrystals of centimeter size, experiments on crack propagation in single quasicrystals are rare. Most of the available experiments are indentation tests where the fracture toughness is estimated from the geometry of the indentations, the applied force and the length of the microcracks that are emitted from the corners [1]. The values for the fracture toughnesses are about 1 MPa $m^{1/2}$ [1, 2], which is close to that obtained for brittle ceramics or silicon.

Cracks in the vicinity of microhardness indentations are observed to propagate predominantly along well defined crystallographic planes [1], suggesting that crack propagation in quasicrystals is, as in periodic crystals, influenced by the plane structure. On the other hand, investigations of cleavage surfaces by scanning tunneling microscopy show that the morphology of fracture surfaces is strongly influenced by the cluster-based structure of quasicrystals [3].

In previous studies [4, 5, 6, 7] we have performed numerical simulations of crack propagation in decagonal model quasicrystals. Decagonal quasicrystals show quasiperiodic order in two dimensions. They consist of quasiperiodically ordered planes which are arranged periodically in the third dimension. For decagonal systems it is thus possible to use simple two-dimensional models to investigate the characteristic features and elementary processes which dominate the fracture of real decagonal quasicrystals.

Icosahedral quasicrystals, however, show quasiperiodic order in three dimensions, which cannot be reduced to simple two-dimensional model systems. In this article, we report on large scale molecular dynamics simulations of crack propagation in three-dimensional icosahedral model quasicrystals.

2 Simulation Method

2.1 Model

The simulations are carried out for a three-dimensional binary model quasicrystal proposed by Henley and Elser [8] as a structure model for icosahedral $(Al,Zn)_{63}Mg_{37}$. As we do not distinguish between Al and Zn, the model consists of two types of atoms, larger ones that represent Mg and smaller ones that represent Al or Zn atoms. The atomic interactions are modelled by Lennard-Jones (LJ) potentials [9], originally derived for the van der Waals type interaction of inert gases. The depths of the LJ potentials are ϵ_0 and $2\epsilon_0$ for atoms of the same and different types, respectively. As unit of length we use the nearest neighbour distance r_0 of two small atoms in the structure. All masses are set to unity, and the time is measured in units of $t_0 = r_0\sqrt{m/\epsilon_0}$. This is thus a very simplistic model quasicrystal, but it nevertheless should produce the correct qualitative behaviour of crack propagation in close-packed quasicrystals like icosahedral $(Al,Zn)_{63}Mg_{37}$.

2.2 Method

Since we are interested in the morphology of fracture surfaces we use a geometry that allows us to follow the dynamics of the running crack for a long time. For this purpose, a strip geometry is used to model crack propagation with constant energy release rate [10]. The samples consist of about 4 million atoms, with dimensions of approximately $450r_0 \times 150r_0 \times 60r_0$. Periodic boundary conditions are applied in the direction parallel to the crack front. For the remaining directions, all atoms in the outermost boundary layer of width $2.5r_0$ remain fixed during the simulation. The strip is homogeneously strained perpendicular to the fracture plane, and an atomically sharp crack is inserted from one short side, to about one quarter of the strip length. 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 does not feel the boundary conditions at the two ends of the strip, so that the dynamics is independent of the crack tip position. The crack thus feels a constant driving force and propagates at constant energy release rate.

The system is initially strained to the Griffith load where the energy release rate G is equal to the surface energy of the two crack surfaces, 2γ. In this work, we will concentrate on exploring brittle fracture without thermal fluctuations. Thus we set the initial temperature to 10^{-4} of the melting temperature T_m, which is close to zero temperature. Afterwards the crack is loaded by adding a fraction of the displacement field to the stable crack. The answer of the system is followed by molecular dynamics simulations. The overloads are given by ΔK^* in the following, which is the relative fraction of the stress intensity factor due to 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 into two regions. Subsequently, the two parts are shifted rigidly by a distance of $10r_0$ perpendicular to the cutting plane. The surface energy is then calculated from the difference of the artificially cleaved and the undisturbed specimen.

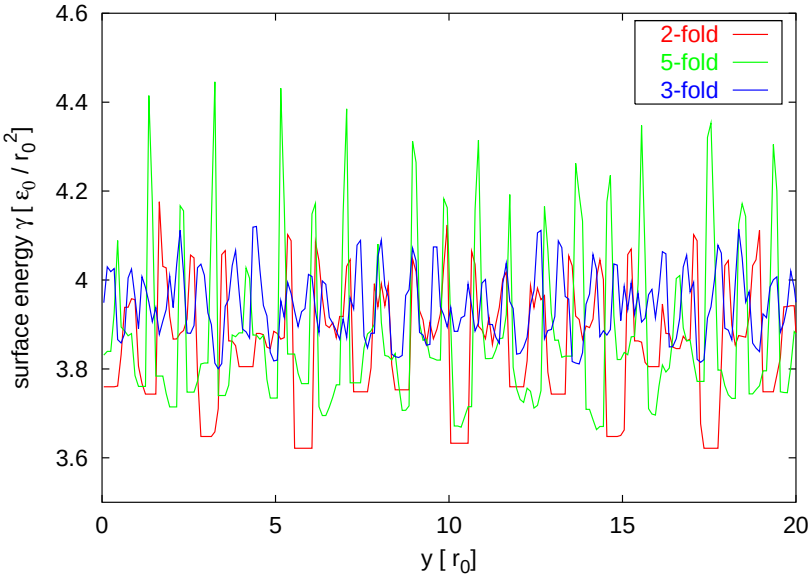

Fig. 1. Surface energy in dependence of the position of the cutting plane, for plane orientations perpendicular to two-, three- and fivefold directions.

For simple crystal structures like the face centered cubic structure of 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. 1 shows the surface energy for three different orientations as a function of the position of the cutting plane. We find a pronounced plane structure of low and high surface energies along twofold directions. The planes of lowest surface energy occur with two separations, forming a Fibonacci chain. Along the fivefold direction the plane structure is less pronounced, but we still find planes of low surface energy, while for the threefold direction there is no such distinct plane structure. For our simulations we select as initial fracture planes surfaces of lowest energy perpendicular to two- and fivefold directions.

All molecular dynamics simulations were done with our own code IMD [11, 12], which performs well on a large variety of hardware, including single and dual processor workstations and massively parallel supercomputers.

2.3 Visualization

There are two essentially different types of data that can be used for the visualization of a molecular dynamics simulation. The first possibility is to compute the distribution of certain scalar quantities like the kinetic energy density, which is evaluated on a regular grid and then displayed with a volume renderer. Fig. 2 shows such a volume data set of the kinetic energy. Regions of low intensity are rendered with high transparency. Sound waves emitted by the propagating crack are clearly visible. In most cases, however, volume data are often too homogenous and show little contrast, so that not much can be seen.

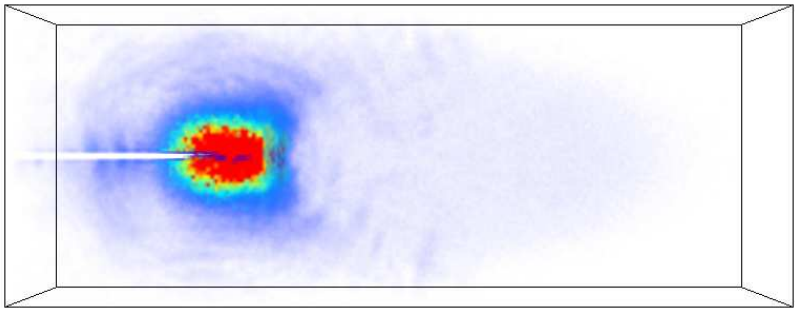

Fig. 2. Kinetic energy density, displayed with the Virvo volume renderer [13]. Sound waves emitted by the propagating crack are clearly visible.

Volume data sets represent, by their very nature, a continuous distribution of some locally averaged quantity. For this reason, they are not suited for the elucidation of microscopic processes. To study crack propagation on an atomistic level, it is necessary to render selected atoms only. Due to the large number of atoms required for the study of crack propagation in three dimensional systems, the selection and reduction of data is of crucial importance. It

is not feasible to always write out the positions of all atoms, and even less to display them all. One simply would not recognize any useful information. In periodic crystals, defects can be visualized by plotting only those atoms whose potential energy exceeds a certain threshold [14]. In quasicrystals, however, atoms may have largely varying local environments. Their potential energy thus varies significantly from atom to atom, even for atoms of the same type in a defect-free sample. Defects can therefore not be visualized by applying a simple energy cut-off as in periodic systems.

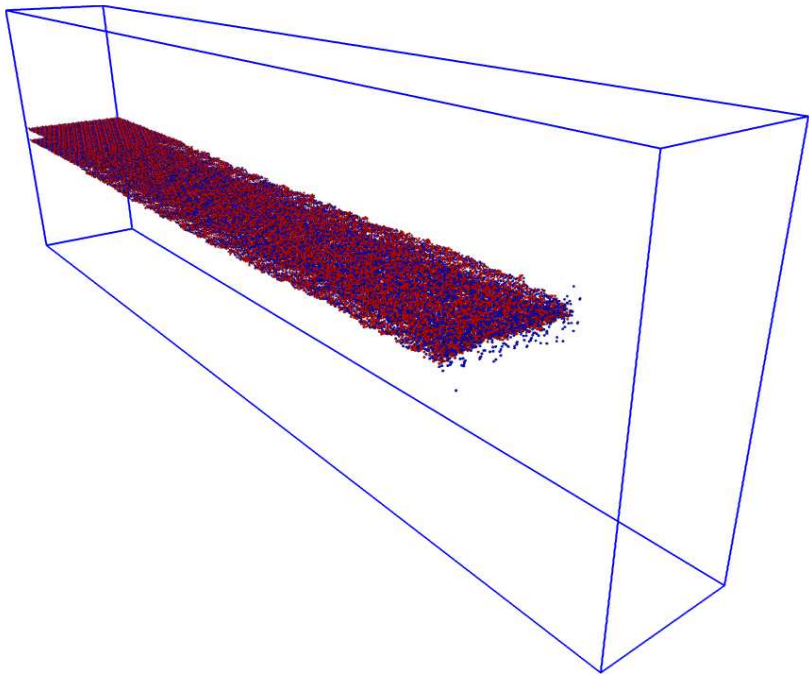

Fig. 3. Snapshot of a simulation with 4 million atoms. Only atoms with low coordination number are displayed.

A more promising method is to display only those atoms whose coordination number is smaller than a certain threshold. The coordination number is evaluated by counting the number of atoms within a certain distance. This cut-off distance is configurable and may depend on the type of the atoms involved. Like the potential energy, the coordination number varies from atom to atom, but to a much smaller degree. In a perfect sample, it is 12 or 13 for the small atoms, and ranges from 14 to 16 for the large atoms. Fortunately, atoms near a defect have a significantly lower coordination number, so that it is possible to visualize fracture surfaces and dislocation cores by displaying only atoms below a suitable threshold in the coordination number. Fig. 3

shows a snapshot of a simulation with 4 million atoms, where atoms are displayed if their coordination number is less than 12 for small atoms, and less than 14 for large atoms. With this method, the number of atoms to write to the output files could be reduced by three orders of magnitude, which allows to take more frequent snapshots instead.

2.4 Online Visualization

In addition to the offline visualization of data written to files during the simulation, an online visualization interface has been developed. A visualization application can request data from the simulation via a socket connection. By the same mechanism, it is also possible to interactively steer the simulation by sending requests to change certain simulation parameters. For online visualization, it is even more important to carefully select the data before it is sent to the visualization. Otherwise, the communication overhead and rendering time could become overwhelming. Currently supported are requests for changing certain simulation parameters, and request for sending selected atoms, along with some of their properties. The selection criteria for those atoms, and the atom properties that shall be sent with them, can be chosen interactively. Atoms can be selected by requesting that their position is inside some rectangular box, and that their type, kinetic energy, potential energy, and number of neighbours are within some chosen interval. All these selection criteria can be switched on and off. The data sent with each selected atom can include the type, the position, the velocities, the kinetic and the potential energy, and the number of neighbours. Each of these quantities can be selected or deselected. This allows to keep the amount of requested data small. The interface can easily be extended, e.g. by requests for sending volume data instead of atom data.

Jürgen Schulze-Döbold of the visualization group at HLRS has written a plugin for the COVER renderer of the COVISE visualization system [15], which implements the protocol sketched above on the visualization side. This plugin can be used for visualizations both on a computer screen and in a virtual reality environment like a CAVE.

The first experience suggests that such online visualization facilities can be a very valuable tool for the rapid determination of suitable simulation parameters. The visualization of large systems in real time requires, however, considerable computational power on the simulation side, which is not always available interactively.

2.5 Performance and Load Balancing

IMD is known to perform very well on PC processors [16]. On a 2-processor Athlon MP1900+ PC, a typical crack simulation run with 4 million atoms takes about 48 hours per 10'000 time steps. Often, some 50'000 to 60'000 time steps are necessary, so that such a simulation takes 10 to 12 days. Since we have

several such machines available, a reasonable throughput can be obtained for parameter studies, but a turnaround time of almost two weeks is not optimal.

As IMD scales very well up to large CPU numbers [16], the solution seems to be massively parallel processing. The only available machine with very many CPUs was the Cray T3E. Its processors are about 8 times slower than the AMD processors on the PCs, however. With 96 T3E CPUs, a simulation run takes some 8 hours per 10'000 time steps. The problem here is, that the maximal time limit of the queues is 12 hours, so that a simulation of 60'000 time steps has to be split into 4 consecutive runs, where the later runs require the output of the previous ones as input. In principle, it is possible to start the later runs automatically from the previous ones, but such a scheme is complicated and error prone. Starting the later runs by user intervention means a lot of work and reduces the turnaround time considerably. The entire simulation would fit into a single run only if about three quarters of the machine could be used, but so many processors are usually not available. With only 96 or 128 CPUs, the restarting of the jobs is sufficiently inconvenient, that most of the simulations have actually been performed on our 2-CPU PCs. The T3E has mainly been used for the shorter relaxation runs which fit into the 12 hour queue limit. It would be highly desirable to reduce the turnaround time considerably, but this seems possible only with a more powerful machine and/or larger queue time limits. In a sense, the problems we want to study have become too large for the T3E.

If a large number of CPUs is used for a crack simulation, the load balancing problem deserves particular attention. IMD uses a geometric domain decomposition scheme for the work sharing [11]. More than 95% of the time is spent in the force computation, which depends on the number of neighbours of an atom. In a crack simulation, fixed boundary conditions are used in two directions, and periodic boundary conditions in the third direction. Atoms near fixed boundaries have less neighbours, so that the corresponding CPUs have less work to do. A similar effect occurs in the middle of the sample along the crack. On the other hand, by the widening of the crack some atoms are moved to the boundary CPUs, which means more work for them. In practice, it is very hard to arrange things such that these competing effects exactly cancel each other. If some CPUs have less work to do than others, they have to wait (at least once every time step) until the other CPUs catch up. This usually occurs in a collective communication routine, or in the collecting of the forces from the neighbouring CPUs. It turns out that for a crack simulation the problem of an unbalanced work load can mostly be avoided by a clever choice of the dimension of the CPU grid. In a normal bulk simulation, it is usually most efficient to assign to each CPU a block of material that is approximately cubic. This reduces the surface of the block, and thus the communication overhead. In a crack simulation, it is more efficient to use only two CPUs in the direction perpendicular to the crack surface. With such a scheme, all blocks contain a similar amount of work, so that the communication overhead (including waiting time) is reduced to as little as 3-4%. If

three or four CPUs are used in this direction, which would result (at a fixed number of 96 CPUs) in a better aspect ratio of the blocks, the communication overhead is increased up to 10-12% (which seems still acceptable).

3 Results

For our simulations we have set up initial fracture planes perpendicular to five- and twofold axes. For both orientations a plane of lowest surface energy is chosen, that corresponds to one of the deepest minima in Fig. 1. The propagation direction is along a twofold symmetry axis. In both cases we have performed a series of simulations with overloads in a range from $\Delta K^* = 0.1$ to $\Delta K^* = 0.8$.

We observe brittle fracture without any crack tip plasticity irrespective of the orientation of the fracture plane. This is in good agreement with simulations of dislocation motion in the same model [17]. These simulations show clearly that the plasticity is very limited in this model, in particular at low temperatures.

For small overloads up to $\Delta K^* = 0.2$, the crack propagates only a few atomic distances r_0, and then stops for all orientations of the fracture plane. The minimal velocity for brittle crack propagation is about 10% of the shear wave velocity v_s. For loads $\Delta K^* > 0.2$ the velocity increases monotonically with the applied load. The crack velocities are in a range of 10-45% of v_s.

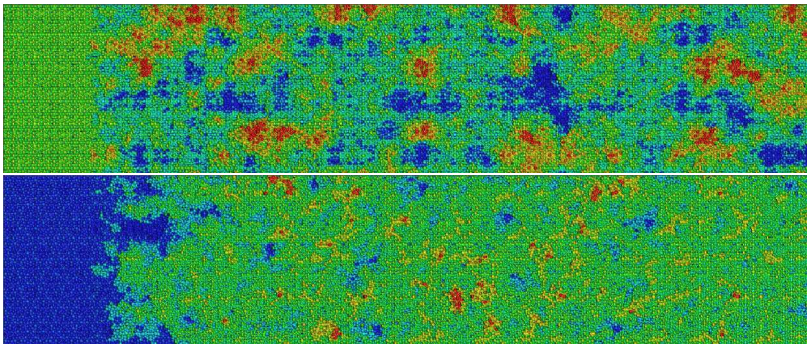

Fig. 4. Height profile of fracture surfaces perpendicular to twofold (top) and fivefold (bottom) axes, for $\Delta K^* = 0.6$. The height increases from blue ($-2r_0$) via cyan ($-1r_0$), green (average height), and yellow ($+1r_0$) to red ($+2r_0$).

To analyse the morphology of the fracture planes, the height of the fracture surfaces, $h(\mathbf{r})$, is calculated as a function of the two lateral coordinates $\mathbf{r} = (x, y)$. Fig. 4 shows examples of such surface profiles. The crack propagation direction is from the left to the right. The initial fracture surface is flat, as can be seen from the homogeneous regions on the left. The surfaces resulting

from the propagation of the crack, however, show a pronounced pattern of regions with different heights. The average vertical roughness is of the order of $4r_0$.

4 Conclusions

In this article we have reported on molecular dynamics simulations of crack propagation in icosahedral model quasicrystals. For this purpose the quasicrystal stucture was endowed with an atomically sharp crack on fracture planes perpendicular to five- and twofold directions. Subsequently the crack was loaded by linear scaling of the displacement field of the stable crack, and the response of the system was followed by molecular dynamics simulations. For both directions we find brittle fracture with rough fracture surfaces.

Acknowledgements

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