# Shock waves in quasicrystals

Johannes Roth

*Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Germany*

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**Abstract**

Shock waves represent a heavy load on materials. In solids they create a variety of defects like shear bands or crystal domains. Waves of large amplitude may destroy the structural order completely. We study shock waves in an Al-Cu-Li-type model quasicrystal, in a closely related crystal structure, the C15 ($MgCu_2$) Laves phase, and in an amorphous solid. If we take the slightly different composition and binding energy into account we find that the sound velocity in all the structures is about the same. If the shock waves are weak, only point defects occur. With increasing intensity we observe broad defect bands in the crystal and the quasicrystals if the cross section of the sample is large enough. Otherwise the structure looks like an amorphous state. At large shock wave intensities the shock front velocity approaches the universal material-independent behavior. The structure is destroyed completely in this regime. The crystal occurs to be slightly more stable than the quasicrystal which means that defects and destruction of the sample are found at higher shock wave intensities.

*Keywords:* Quasicrystals; Shock Waves; Al-Cu-Li; C15 Laves phase

## 1. Introduction

Quasicrystals differ in many aspects from ordinary crystals as a result of their aperiodicity. The nonexistence of Brillouin zones for example leads to a backscattering of plane waves at any wave number and to the opening of energy gaps. Phonons are hindered on propagation through a sample and heat conductivity is reduced. On the other hand the close packing of atoms leads to an averaging effect like in amorphous system and to a restoration of the behavior predicted by continuum theory for the long-range limit.

Shock waves are a nice tool to expose a solid to highly uniaxial stress and to introduce defects without explicitly constructing them. In a monatomic crystal the shock stress is relaxed to a energetically more favorable hydrodynamically compressed state by slippage. Often stacking faults are created which permit an easy detection of the slippage. For a crystal it would be rather easy to construct slip planes and stacking faults and to analyze them. This is not the case for quasicrystals. If geometric constructions are used, complicated and rather arbitrary procedures have to be carried out to produce for example dislocations associated with extended defects [1]. This can be avoided if we use shock waves. Here the system itself choses the defect planes and the Burges vectors.

Our first goal in this study is to find out whether quasicrystals behave different than other materials if they are penetrated by shock waves. Metals and alloys as well as fcc model crystals show a rather universal behavior with respect to the shock front velocity for example. We observe that this behavior is also valid for quasicrystals binary crystals and binary amorphous solids in the case of strong shock waves. For weak shock waves a deviation from the universal behavior is observed, and a difference between the crystal and the quasicrystal is showing up.

Our second goal is to find out if new kinds of defects occur in the quasicrystal. By definition, a real shock wave in a crystal (as opposed to a very strong elastic wave) causes a permanent plastic deformation. Usually one finds stacking faults caused by slipping or twinning and martensitic deformations. In a quasicrystal these defects can occur also, but additional types of defects are possible: phason flips,

phason walls, or transformations to crystals and approximants. It turns out that the types of defects in the quasicrystal are indeed different from those of the monatomic crystal, but similar to the binary crystal.

We will first describe the simulation setup and the structure model. We will then review shortly the general behavior of shock waves. The next sections contain the results and the discussion.

## 2. Generation of the Shock Waves and Simulation Setup.

Shock waves have been generated in three-dimensional quasicrystals of the closed-packed Frank-Kasper-type which is realized in the Al-Cu-Li icosahedral quasicrystals. The structure can be regarded as a quasiperiodic arrangement of oblate and prolate rhombohedra decorated with small $A$ atoms at the corners and edge centers [2]. The large $B$ atoms divide the diagonal of the prolate rhombohedron in the fraction $\tau$:1:$\tau$, with $\tau$ the golden mean $(1+\sqrt{5})/2$. For comparison, simulations in a related cubic crystalline model, the C15 Laves phase of $MgCu_2$, have been carried out. The crystal phase can be regarded as a low-order approximant of the quasicrystal build of the prolate rhombohedra only. An amorphous solid was generated from the Laves crystal by melting, equilibrating and quenching. The three structures have a rather similar composition: The crystal and the amorphous solid have the structure formula $A_2B$, the composition of the quasicrystal is $A_{0.764}B_{0.236}$. The interactions were modeled by Lennard-Jones potentials. The radii of the potential minima have been adjusted to the shortest $AA$, $AB$ and $BB$ distances. The depth of the potentials between atoms of the same type is $-\epsilon$ and is $-2\epsilon$ between atoms of different types. The binding energy is $11.485\epsilon$ for the quasicrystal, $12.974\epsilon$ for the crystal, and 10.564 for the amorphous solid.

There are a number of well established methods to generate shock waves in computer simulations [3]. In our case we have cut the sample into two halves and moved the two parts against each other at constant velocities $\pm u_p$. Two shock waves are generated at the center of the sample and move through the sample at velocities $\pm(u_s - u_p)$. The setup is equivalent to a piston compressing a sample at rest at speed $u_p$, thereby creating a shock wave at speed $u_s$.

For the simulations we have used the IMD molecular dynamics simulation program developed at our institute [4]. This program can be run on workstations as well as on massively parallel computers.

The samples sizes ranged from 20,000 to about 1,000,000 atoms. The geometry was a long rod with cross-sections 14×14, 23×23, and 61×61 in units of the minimal atomic distance and lengths 100, 160 and 260. The boundaries were open along the shock wave propagation direction and periodic along the two transverse directions. For the amorphous solid we used samples with 80,000 atoms and size 160×14×14.

After the samples have been generated they are equilibrated for a time interval of $t = 10a\sqrt{m/\epsilon}$ ($a$ is the smallest interatomic distance and $m$ the mass of the atoms) at $kT = 0.001\epsilon$ and pressure $P = 0.01\epsilon/a^3$ to prevent a singular behavior of the shock waves as explained in the next section.

## 3. General Remarks on Shock Waves

Shock waves have been studied by computer simulation for quite some time [5]. In liquids stable shock waves with a steady profile exist. This can be derived from the Navier-Stokes equations and has been confirmed by computer simulations and experiments.

For solids the results have been rather controversial for a long time, until Holian [6] could finally clear up the case: there were claims that no steady shock waves exist [7] even in more-than-one-dimensional crystals. Today it is known that there are no steady shock waves in one dimension due to the missing transverse direction which would permit equilibration. In two and three dimensions the behavior is one-dimensional if either the temperature is set to zero or the shock wave intensity is too low.

A convenient measure for the intensity is obtained if the piston velocity is given in terms of the longitudinal sound velocity $c_0$ at zero pressure and zero temperature. For fcc crystals we find the crossover from one- to three-dimensional behavior at about $u_p/c_0 = 0.5$. At about $u_p/c_0 = 1$ the shock wave melts the sample. A diagram of $u_s$ vs. $u_p$ is called a Hugoniot plot. The velocity of the shock front is $u_s/c_0 = 1.86 \cdot u_p/c_0 + 1.01$ [3]. It turns out that the constants of the linear relation between $u_s$ and $u_p$ are rather universal. The slope is between 1.6 and 2.0 for a broad variety of sufficiently anharmonic interactions [8]. It is determined by the repulsive part of the interaction. The same values of the slope are obtained for all kinds of metals and alloys in experiment. The theoretical formulation of this relationship requires two ingredients: the Rankine-Hugoniot relations which can be derived from the conservation laws of energy and momentum and the continuum equation, and a simple Grüneisen equation of state which is valid for all shocked materials [9].

Due to the wide-range validity of the Hugoniot relation we would expect that it is also true for binary crystals and quasicrystals. A simple demonstration is possible for a one-dimensional chain of atoms of equal mass [8]. The shock wave velocity can easily be derived for atoms of diameter $\sigma$ and spacing $a$ with the help of a distance-time diagram. If the per-

iodic arrangement is replaced by a Fibonacci chain or even a random arrangement of the atoms of the *same* density we find that the shock front velocity has always the same value $u_s = 2/(1-\sigma/\overline{a}) \cdot u_p$ where $\overline{a}$ is now the average distance between the atoms.

## 4. Results

Fig. 1 displays the results of the Hugoniot plot for Laves crystal and quasicrystal. We have not computed the longitudinal sound velocity explicitly but have assumed that it is the value of $u_s$ at $u_p \to 0$ as in the monatomic crystalline cases mentioned above. For the quasicrystal we obtain $c_0 \approx 12\sqrt{\epsilon/m}$, for the crystal $c_0 \approx 14.5\sqrt{\epsilon/m}$ and for the amorphous solid $c_0 \approx 10\sqrt{\epsilon/m}$. Since the relation between the sound velocities is about the same as the square root of the relation between the binding energies and the unit of velocity is $\sqrt{\epsilon/m}$ we conclude that the speed of sound is about the same for all three structures. A more precise comparison of the sound velocities would require a direct computation of the speed of sound.

At low piston velocities we observe unsteady shock waves, a deviation from the universal behavior, and different slopes for crystals and quasicrystals. The slopes are 3.1 for the crystal and 2.6 for the quasicrystal. This result is independent of the starting temperature of the sample. Between 0.3 and 0.6 $u_p/c_0$ we find the crossover from the one-dimensional to the three-dimensional case of strong shock waves. At higher piston velocities we recover the universal behavior. In the case of the amorphous solid we observe the universal behavior for all shock front velocities. But in the whole range from $u_p/c_0 = 0$ up to $u_p/c_0 = 1$ we find that the *initial* shock front velocities lie on the straight line of the one-dimensional case. After a simulation time of $t = 0.05a\sqrt{m/\epsilon}$ a transition to the three-dimensional case occurs. Thus it takes only a short time for the sample to develop a steady shock wave. The $u_s$ vs. $u_p$ curve obtained in our simulations does not depend on the sample cross-section and on the length of the rod as long as the shock wave has not penetrated the whole sample during simulation time.

In the crystal the crossover from the one-dimensional to three-dimensional behavior occurs at shock wave intensities higher than in the quasicrystal. The reason is that the local symmetry around an atom is on average larger in the crystal than in the quasicrystal, and the transition to the universal behavior is a symmetry breaking in such a way that a coupling between the normal and the transverse directions has to be established. This occurs through the random fluctuations caused by temperature.

The crystal structure remains largely perfect up to $u_p/c_0 \approx 0.37$. Only diffusion is observed. Within

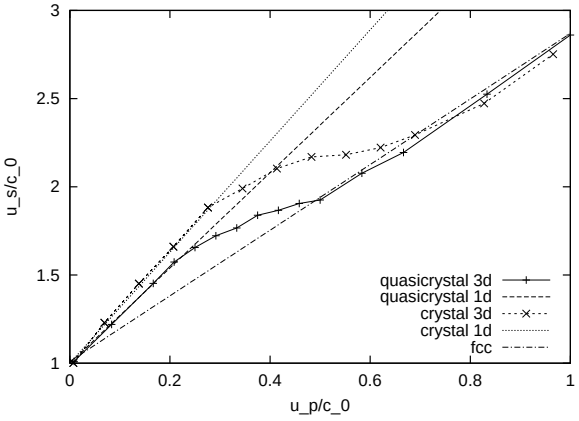


Fig. 1. Hugoniot plot of the shock velocity versus piston velocity. At low shock wave intensities and at the beginning of the simulations we observe the one-dimensional behavior, indicated by the straight lines. Between $u_p/c_0 = 0.3$ to 0.6 we find the crossover to the three-dimensional shock mode and the change of the slope to the universal value. The results for a simple fcc crystal are given for comparison [3]. The curve for the amorphous solid coincides with the fcc curve.

a short interval of about $u_p/c_0 = 0.1$ the behavior changes strongly. Defect bands occur which perfect crystalline domains. The bands grow with increasing strength of the shock wave, and finally only a few crystalline spots are left. Starting at $u_p/c_0 \approx 0.5$ the structure becomes destroyed completely by the shock wave.

The quasicrystal stays intact up to a piston velocity of about $u_p/c_0 = 0.25$. Only diffusion processes occur in this regime. Between $u_p/c_0 = 0.25$ and 0.55 defect bands are observed as can be seen in Fig. 2. The clumps are the intersections of the defect bands which run diagonally through the sample. At shock waves stronger than $u_p/c_0 = 0.55$ the quasicrystal becomes amorphous.

The defect bands are different from ordinary stacking faults which have a typical width of a monolayer. The width of the bands is up to 10 interatomic distances $a$ and the separation of the order of 35 $a$. The spacing between the bands depends on the cross section of the sample since the network of defect bands is generated by the periodic boundary conditions. In the case of small cross sections the boundary conditions may even mimic an amorphous state. Only for very large simulation cells [3] it was possible up to now to distinguish different slipping systems.

In the amorphous solid there is on distinction between different regimes. No defect bands occur, and the system behaves like a structureless fluid.

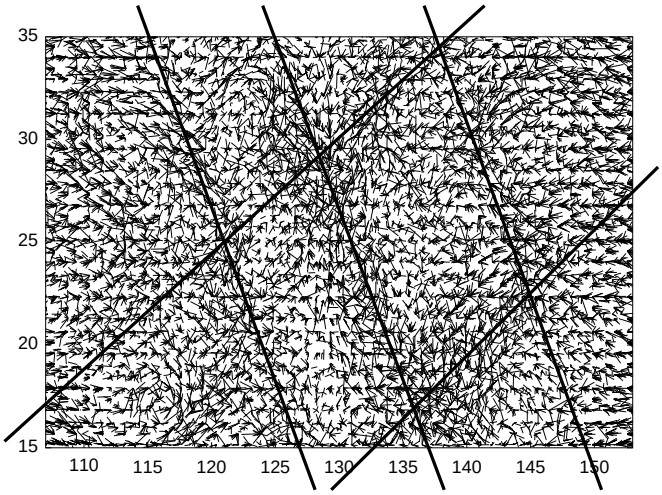


Fig. 2. Pattern of defects in the quasicrystal at $u_p/c_0 = 0.45$. The clumps are the intersections of the diagonal defect bands indicated by the bars through the figure. A picture of the crystal would look wuite similar.

## 5. Discussion

We have demonstrated that there is no deviation from the universal Hugoniot law for shock front velocities in a binary crystal alloy and in a two-atomic quasicrystals in the case of strong steady shock waves. In the case of weak shock waves, however, we find that the slopes for the quasicrystal as well as the crystal differ from the Hugoniot law. The reason is the one-dimensional behavior of the system. The difference between the slopes of the crystal and the quasicrystal may be an effect of the aperiodicity.

In the quasicrystal we have found defect bands similar to the shear bands observed in fcc crystals [3]. Up to now it has not been possible to characterize them more precisely. It can even be speculated that the structures are melted locally. The defect bands could not be observed if the transverse dimension of the samples was too small. It will be necessary to carry out simulation with larger samples to reduce the influence of periodic boundary conditions which fold the defect bands back onto themselves.

We have tried to find a crystal and a quasicrystal structure which are as close as possible. There are still differences between the average binding energies and the composition, however. Therefore we can not rule out that some of the effects observed (for example the different slopes in the Hugoniot plot) are due to the structural differences.

The propagation direction of the shock waves was the four-fold direction in the crystal, and the two-fold direction in the quasicrystal which is normal to the close-packed planes. It is planned to extend the simulations to the other symmetry directions to find out whether differences exist.

The crystal and the quasicrystal structure remain fully intact in the weak shock wave regime, but here the shock waves are not "real" shock waves since they do not cause plastic deformation. In the intermediate range we observe complicated defect structures. In the strong shock wave regime both structures are destroyed, in contrast to simple crystals. The reason is that it is not possible in our model to exchange $A$ and $B$ atoms at random without destabilizing the structure. Therefore many defects which are permitted in monatomic structures are fatal for binary structures.

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## References

[1] G. Schaaf, J. Roth, H.-R. Trebin, Numerical simulations of dislocation motions in an icosahedral quasicrystal, this volume.

[2] J. Roth, R. Schilling, H.-R. Trebin, Stability of of monatomic and diatomic quasicrystals and the influence of noise, Phys. Rev. B **41** (1990) 2735.

[3] B. L. Holian, P. S. Lomdahl, Plasticity induced by shock waves in nonequilibrium molecular dynamics simulations, Science **280** (1998) 2085.

[4] J. Stadler, R. Mikulla, H.-R. Trebin, IMD: A software package for molecular dynamics studies on parallel computers. Mod. Phys. **C** (1997) 1131. The home page of IMD can be found at www.itap.physik.uni-stuttgart.de/~imd.

[5] B. L. Holian, Atomistic computer simulations of shock waves, Shock Waves **5** (1995) 149.

[6] B. L. Holian, Modeling shock-wave deformation via molecular dynamics, Phys. Rev. A **37** (1988) 2562.

[7] D. H. Tsai, R. A. MacDonald, An atomistic view of shock wave propagation in a solid, High Temp. High Press. **8** (1976) 403.

[8] B. L. Holian, G. K. Straub, Molecular dynamics of shock waves in one-dimensional chains, Phys. Rev. B **18** (1978) 1593.

[9] M. H. Rice, R. G. McQueen, J. M. Walsh, Compression of solids by strong shock waves, in: F. Seitz, D. Turnbull (Eds.), Solid State Physics, Vol. 6, Academic Press, New York (1958), p.1.