Dislocations in quasicrystals and their interaction with cluster-like obstacles

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A dislocation moving through a quasicrystal leaves in its wake a fault denoted phason wall. For a two-dimensional model quasicrystal the disregistry energy of this phason wall is studied to determine possible Burgers vectors of the quasicrystalline structure. Unlike periodic crystals, the disregistry energy is an average quantity with large fluctuations on the atomic scale. Therefore the dislocation core structure and mobility cannot be linked to this quantity e.g. by a Peierls-Nabarro model. Atomistic simulations show that dislocation motion is controlled by local obstacles inherent to the atomic structure of the quasicrystal.

In the last five years it has become possible to grow thermodynamically stable quasicrystals of high structural quality and sizes which have allowed one to measure properties like plasticity and fracture. The data have initiated a wealth of studies, in which the influence of quasiperiodicity on physical properties is being explored. Simultaneously, potential applications of quasicrystals have been discussed, for example as friction reducing, oxidation resistant, non-adhesive coatings, as solar converters or for hydrogen storage.

The structure of quasicrystals is also responsible for special mechanical properties. On this subject an impressive set of experimental results is available: i) At room temperature quasicrystals are hard as silicon and extremely brittle. ii) At about 80% of the melting temperature they become plasticly deformable up to 30% and soften upon straining. iii) Stress relaxation experiments reveal unusually high values for the activation enthalpy and for the activation volume. iv) For AlMnPd it has been proven that the deformation is governed by dislocation motion.

In this letter we provide atomistic insight into the mechanical behavior of quasicrystals. It will turn out that two structural features govern the motion of dislocations: the faults in the wake of dislocations and cluster-like obstacles in the glide planes.

Quasiperiodic structures can be obtained as cuts of an irrationally oriented n-dimensional hyperplane (physical space) through a d-dimensional periodic crystal, where d > n is the number of incommensurate length scales. Due to the periodicity of the hyper-crystal, dislocations also exist in quasicrystals. The d-dimensional Burgers vectors carry an n-dimensional component b∥ in physical space and a (d − n)-dimensional component b⊥ in the complementing orthogonal space. Moving a dislocation in a two-dimensional quasicrystal leaves in its wake a phason-wall, separating two areas with a phase difference b⊥, which gives rise to faults in the pattern and therefore differences in the atomic environments compared to the perfect quasicrystal. Atomic jumps move these faults and the wall may consequently vanish by diffusive processes.

Recently, we performed numerical simulations of plastic deformation on a two-dimensional binary model quasicrystal displayed in Fig. 1. We observed that the phason-wall remained sharp at low temperatures. But close to the melting temperature it was broadened by strain-induced diffusion and developed into a several bond-lengths wide glide zone, on which secondary dislocation dipoles were forming. Since this feature may be the central mechanism for the strain softening, we further study the phason-wall here. We calculate and discuss the “disregistry energy”, which is the potential energy necessary to shift one half of a quasicrystal rigidly over the other along a glide plane (line in two dimensions). Based on the smallest displacement that provides a minimal disregistry energy, we construct a generic dislocation by applying a kink-like displacement field. We then investigate the dislocation core structure, the friction force impeding dislocation motion, and the (Peierls) stress to overcome it.

We use the same binary model quasicrystal as in previous shear simulations. The model originates from the decagonal Tübingen tiling of the plane by acute and flat triangles. The vertices are occupied by large (A) atoms. Small (B) atoms are placed in the interior of the acute triangles. In Fig. 1(left) the system is depicted in the atom representation, in Fig. 1(right) in the bond representation, where next neighbors of different atomic type are connected. The model is stabilised by Lennard-Jones potentials. The potential depth is taken as 1 (LJ-unit) for AA and BB bonds, and as 2 for AB bonds in order to avoid phase separation. The LJ unit of length is one AB bond.

A striking feature of the structure are concentric rings of ten small and ten large atoms. Due to the large number of energetically favorable AB-bonds these rings are tightly bound and resemble the cluster structure of real systems. The simple model used here therefore reproduces the two most important characteristics of real quasicrystals: namely quasiperiodicity and clusters. The clusters are arranged on families of parallel lines of two separations which form a Fibonacci sequence. The space
in between the large separation is traversed by a straight line (dashed line in Fig. 1) which does not touch any clusters. This line is characterised by a low surface energy 1 and serves as an “easy” path for dislocations 1. Equivalent families of lines result from rotations by 36°.

The unrelaxed disregistry energy along such a plane is displayed in Fig. 2 (in LJ units). For periodic crystals this energy 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, because the spectral decomposition for the spatial frequencies shows the values 1 and the inverse golden mean \( \tau^{-1} = (\sqrt{5} - 1)/2 \).

There are two classes of local minima in the disregistry energy. Those of the first class are very deep, with values of the order of \( 10^{-4} \) (vertical thin lines in Fig. 3). The positions of these minima are projections \( b_1 \) of low indexed hyper-crystal lattice vectors \( b \), whose orthogonal component is within the acceptance domain of the triangle tiling. Therefore they are tiling vectors and represent the primary Burgers vectors of our model. The small but finite value of the minimum is the energy of the phason wall for phase difference \( b_\perp \).

In between there are minima of a second class. Their corresponding values \( b_\perp \) are outside the acceptance domain, and the lengths \( b_\parallel \) do not belong to the triangle tiling. The energies of the minima are monotonically (but not linearly) correlated with \( |b_\perp| \). The disregistry energies of the second class of minima are therefore much higher, of the order of 1. Elastic relaxation reduces this value to \( E_{ph} \approx \frac{1}{2} \).

In principle, the \( x \)-axis is densely covered with projections \( b_\parallel \) of lattice vectors \( b \). Therefore, a dislocation always can split into others of smaller Burgers vectors \( b_\parallel \). However, these necessarily have larger \( b_\perp \) components and consequently lead to a high disregistry energy. Such dislocations of high phasonic component will therefore be connected by a high energy phason wall which will prevent them from splitting.

Since a moving dislocation necessarily creates a phason wall with finite phase difference \( b_\perp \) and finite disregistry energy, it is interesting to note that such a fault will be a preferred region for the generation of further dislocations, which then reduce the disregistry energy.

In periodic crystals a Frank-Read \([15]\) source produces a sequence of dislocations with the same Burgers vector. In a quasicrystal such a source would accumulate a phase difference \( n \cdot b_\perp \), \( n \) being an integer, in the glide plane of the emitted dislocations. As the stacking fault energy rapidly increases with \( b_\perp \), the source cannot operate continuously with a constant Burgers vector. Instead the dislocation should split into two with smaller \( b_\parallel \) and higher \( b_\perp \). Only \( b_\parallel \) components which correspond to the low lying minima in Fig. 2 should actually be emitted, while the part of the initial Burgers vector which would create the high energy phason-wall should be left at the location of the source \([14,16]\). Consequently, we predict that a Frank-Read source in a quasicrystal will not emit identical Burgers vectors but Burgers vectors of varying length \( b_\parallel \). It is obvious that the source will also have to emit Burgers vectors with larger \( b_\perp \) components. This result is in agreement with recent experimental observations \([15]\) that the probability of dislocations with larger \( b_\perp \) components increases with plastic strain.

Due to the homogeneity in local surroundings, in periodic crystals the (global) disregistry energy resembles the local potential for a dislocation \([14]\) and hence has been successfully applied by Peierls \([20]\) and Nabarro \([21]\) for a model of the dislocation core structure. In quasicrystals there are many different atomic neighborhoods. The disregistry energy is an average over the total glide plane. The large local fluctuations can invalidate any reasoning about the dislocation core structure and mobility drawn in analogy to periodic crystals. This observation is explored by direct atomistic simulations of dislocation cores.

In physical space a dislocation with phason wall was constructed by imposing a kink-like displacement field of total displacement \( b_\parallel = 1.9 \) (see Fig. 3) on a long slab of the binary model. The slab had a total length of 300 AB interatomic spacings and an aspect ratio of 5. The dislocation was placed on a easy glide plane in the center of the sample. After relaxation we imposed homogeneous shear strains between 1% and 3%. To fix the deformation on the upper and lower boundary, the atoms were arrested in a strip four AB interatomic spacings wide. The evolution of the system then was studied with a constant energy molecular dynamics procedure from an initial temperature of \( 10^{-6} \) times the melting temperature. We calculated the displacement field with respect to the defect free initial configuration parallel to the slip plane and analyzed snapshots of the atomic sites taken from the simulation.

Fig. 3 shows the horizontal components of the displacement field parallel to the slip plane for shear deformations of 1%, 2% and 3% at different timesteps. At applied strains of 1% and 2%, there is no motion of the dislocation as a whole. Instead, it remains sessile and splits into two dislocations with \( b_1 = 1.1 \) and \( b_2 = 0.8 \), which corresponds to the first secondary minimum in Fig. 2. An increase of the deformation from 2% to 2.5% doubles the separation of the two dislocations. This observation is a first indication that not the stacking fault energy, i.e. the attractive force between the cores of the partials, but local obstacles dominate their separation.

An increase of the applied shear deformation to a value of 3% leads to dislocation motion over the total length of the strip (third diagram in Fig. 3). After 5000 time steps the dislocation is split in two dislocations similar to the simulation at 2% shear. Both then proceed individually with varying velocity and an oscillating splitting length until the dislocation reaches the boundary of the system.

Our simulation therefore suggests a value of the Peierls stress between 2.5% and 3% of the shear modulus \( G \). It is the same order of magnitude as the value calculated for
BCC transition metals\cite{13} which show brittle cleavage fracture at low temperature. The Peierls stress for a periodic triangular lattice with a similar interaction model is about 100 times lower\cite{22}. Thus our calculations result in a physically reasonable value of the Peierls stress for a brittle material like a quasicrystal.

Again we conclude that local obstacles on the glide plane dominate the dislocation motion since both dislocations moved neither at constant velocity nor with constant separation. In the following we will illuminate the microscopic nature of the structure intrinsic obstacles observed in our system.

All simulations performed in this context indicate that the atomic environment highlighted in Fig.\ref{fig:diagram} plays the role of a local obstacle for dislocation motion. Here one large (A) atom on the upper part is bound to five small (B) atoms below the glide plane. This is a highly coordinated atomic cluster, which has the largest accumulation of bond energy along the "easy" plane. In Fig.\ref{fig:diagram} a dislocation stops in front of such an obstacle. In all calculations up to strains of 2\% an elastic repulsion between the dislocation core and the atomic environment on the glide plane with the highest coordination was observed. At higher strains, in some of our calculations, the leading dislocation core destroys the obstacle described above and transforms it into a nonplanar configuration which again is sessile. The dislocation is able to cut the obstacle only if the strain is increased beyond the Peierls stress.

If the surmounting or cutting of these intrinsic obstacles is the rate limiting step in dislocation motion, the size of the obstacle may also explain the high activation volume for dislocation motion\cite{23} and has indeed been proposed to do so\cite{23}. Furthermore, it is worth mentioning that an atomic cluster which is cut by the first dislocation is a much weaker obstacle for a second dislocation. Thus the cutting of the obstacles may even explain the strain softening which has been observed experimentally\cite{23}.

Although the binary quasicrystal model used in this paper is very simplistic, it reflects the most important features of real quasicrystals, i.e. quasiperiodicity and clusters and therefore permits us to reach conclusions relevant and transferable to real quasicrystals. The disregistry energy of the phason wall leads to the identification of true Burgers vectors whose phason wall energies are at least one order of magnitude lower than the relaxed phason wall energy of these dislocations of the second kind. These Burgers vectors have varying length and, consequently, a Frank-Read source should produce more than one dislocation type in a quasicrystal.

Atomistic simulations were performed to calculate the stress which is necessary to move a dislocation. Its minimal value, the Peierls stress, is of the order of magnitude of other brittle materials like BCC transition metals. However, our simulations reveal the dominating role of highly coordinated atomic environments as structure intrinsic obstacles for the dislocation motion. The interaction between dislocations and these obstacles is currently being studied in more detail with more realistic three-dimensional models.

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Although Frank-Read sources have been observed in quasicrystals by in-situ transmission microscopy [23], they do not necessarily represent the most common sources of dislocations.

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FIG. 1. Binary tiling obtained from the Tübingen triangle tiling by decoration. Left: Atoms are displayed as disks (atom representation). Right: Bonds are drawn between different atomic species (bond representation). The ten-pronged stars represent tightly bound clusters and are arranged on families of planes (full lines). The easy planes (broken line) run in between the full lines of large separation.

FIG. 2. Disregistry energy along the easy plane of Fig. 1. For each minimum the orthogonal component \( b^\perp \) of the Burgers vector is indicated. \( E_{\text{rel}} \) is the energy for the relaxed phason wall corresponding to the second minimum. Lengths and energies are in LJ units.

FIG. 3. Displacements parallel to the slip plane of a dislocation at an applied shear strain of 1%, 2% and 3% and for different times.

FIG. 4. Section of a configuration obtained after 50000 time steps at a shear strain of 2%. Both partials are framed by Burgers circuits. The Burgers circuit around the leading partial is repeated in the undisturbed material below to visualize the Burgers vector. The atoms of the environment which acts as an obstacle for dislocation motion are drawn as disks. The glide plane is marked by a line.