

PEAK BROADENING IN QUASICRYSTALLINE SOLIDS

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ABSTRACT: We investigate the response of perfect quasiperiodic and orientation-preserving random structures when their bonds are perturbed homogeneously. We find that the perfectly quasiperiodic networks are stable against such perturbations while the (translationally) disordered structures exhibit significant accumulation of strain. These grown networks are characterized by root-mean-square (rms) phason fluctuations which grow linearly with system size and exhibit strain accumulation which also grows linearly with system size. Furthermore, we find a dependence of strain accumulation on cooling rate.

Defects in quasiperiodic structures, called phasons, have been introduced in order to account for the broad diffraction peaks and distorted

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diffraction patterns observed in scattering experiments on quasicrystals. Also, orientation-preserving random structures^{1-4]} have been introduced in order to account for these features. More specifically, phason strains are created during the growth process. Shifts of the scattering peaks are due to the linear component of the phason strain while peak broadening is due to the nonlinear modulations. In this paper, our definition of the word "quasicrystal" corresponds to the experimental one, *i.e.* a solid having a sharp but non-crystallographic diffraction pattern. In addition to quasiperiodic structures this definition includes random aggregation models^{1-4]} such as the icosahedral glass. The two dimensional analog of these systems has been observed experimentally by different groups.^{5]}

We have followed^{1]} the standard approach to study strain accumulation in solid mechanics: (1) homogeneously perturb a system in order to generate non-zero forces (*i.e.*, stresses); (2) these stresses produce displacements (*i.e.*, strains); (3) for very small strains (10% or smaller) the behavior of most solids is perfectly elastic (*i.e.*, the body recovers its original shape and size after the stress is removed); (4) compute the displacement field, subtracting the average translation and the average rotation, and its root-mean-square average.

The procedure summarized above has been applied^{1]} to about fifty two dimensional (2D) elastic networks by using molecular dynamics techniques. These networks were all different from each other. More specifically, we studied the following aspects of strain accumulation: (a) size dependence (aggregates ranging from 50 to 5000 decagons), (b) perfect quasiperiodic structures, obtained by decorating Penrose lattices, versus several orientation-preserving random structures, (c) relation with the behavior in the phason field, (d) cooling-rate dependence, (e) dependence of the results with the magnitude of the applied stresses, and verification that the structures studied were in the elastic regime, (f) point out recent experimental works which are consistent with our results.

The building blocks of our model are decagons packed edge to edge. These decagons can always be related by a pure translation. Furthermore,

such a translation can always be expressed as an integral linear combination of four basis vectors \mathbf{e}_i^{\parallel} ($i = 1, \dots, 4$). This fact is equivalent to the statement that the possible decagon centers may be obtained by projecting a suitable 4D lattice. Therefore, each decagon is associated with a pair of 2-component vectors: \mathbf{x}^{\parallel} , the location of its center; and \mathbf{x}^{\perp} , its "phason" coordinates. The pair $(\mathbf{x}^{\parallel}, \mathbf{x}^{\perp})$ define a point in a 4D lattice. This procedure is a simple extension of the projection technique used for incommensurate structures. Details of this technique are given elsewhere.^{2]} For our purposes, it is sufficient to note that if the separation (in the physical plane) of two decagons is given by $\Delta \mathbf{x}^{\parallel} = \sum_{i=1}^4 n_i \mathbf{e}_i^{\parallel}$, then $\Delta \mathbf{x}^{\perp} = \sum_{i=1}^4 n_i \mathbf{e}_i^{\perp}$ gives the separation of their phason coordinates.

Our strain-free reference solid is the geometrical structure of edge-sharing decagons. The local structure is constrained by the requirement that the next-nearest-neighbor (nnn) decagon separation is $\tau = (1 + \sqrt{5})/2$ times the nearest-neighbor (nn) or edge-sharing separation, which will be taken as unity. The inclusion of nnn bonds greatly increases the connectivity of the network. We use both types of bonds to stabilize the network mechanically. The original edge-sharing structure, or reference solid, is stabilized by the choice $r(\tau)/r(1) = \tau$ where $r(\tau)/r(1)$ is the ratio of the nnn and nn equilibrium distances between the centers of the decagons. We are interested in the formation of strains, *i.e.* deformation of the reference solid, when $r(\tau)/r(1)$ differs infinitesimally from τ . In this limit, *i.e.* the *elastic* regime, the actual form of the potential is irrelevant since the harmonic behavior dominates the dynamics. A trivial consequence of modifying the potential is a uniform strain, *e.g.* isotropic contraction or expansion, of the unrelaxed packing. The uniform component of the strain was eliminated using the method of least squares. Our samples have a circular shape in order to minimize the ratio of boundary over bulk decagons, thus minimizing boundary effects.

Several works^{6]} have also regarded covalent glasses, like a-Si and window glass, as elastic networks. Of course, glasses, which are either random-packed (*e.g.*, metallic glasses) or covalent, do not exhibit the long-range orientational order present in our packings. However, they all can be described by networks or graphs. The graph for covalent glasses is called a continuous random

network. The vertices of the graph represent the atoms while the edges represent the bonds. This graph, called regular, has a fixed coordination number because the atoms have a fixed chemical valency. In metallic glasses, the edges are defined through the Voronoi partition of space. As in the covalent case, the vertices represent the atoms and the coordination number is four in three dimensions. A central question refers to the origin of the macroscopic rigidity of the network. A proposed answer invokes a harmonic elastic energy which is isotropic, as in rubbers and gels. Another refers to an elastic energy which is invariant under rigid-body rotations, as in solids. The elasticity of covalent networks is often prescribed by a potential energy with a bond-stretching force term, which is central but locally anisotropic, and *also* a bond-bending force term, which involves *next-nearest neighbors* and is responsible for the *rigidity* of the network. Note that these locally anisotropic forces must hold together a disordered material which, macroscopically, is elastically isotropic.

The scattering phase angle is given by

$$\mathbf{G}^{\parallel} \cdot (\mathbf{x}_i^{\parallel} + \delta \mathbf{x}_i) = -\mathbf{G}^{\perp} \cdot \mathbf{x}_i^{\perp} + \mathbf{G}^{\parallel} \cdot \delta \mathbf{x}_i \quad (\text{mod } 2\pi).$$

where \mathbf{x}_i^{\parallel} is the position of the *i*th decagon in the reference solid and $\delta \mathbf{x}_i$ its displacement after relaxation. Several diffraction experiments in quasicrystals^{7,8]} have established a linear growth of peak width with phason momentum \mathbf{G}^{\perp} . The apparent linear growth of $\Delta^{\perp}(R)$ with R , seen also in the 3D icosahedral model,^{4]} is consistent with this behavior. From equation (1), it is clear that fluctuations in both \mathbf{x}_i^{\perp} and $\delta \mathbf{x}_i$ lead to peak broadening. In particular, for peaks with $|\mathbf{G}^{\perp}| \gg |\mathbf{G}^{\parallel}|$ one considers a coherence radius R_c defined by

$$|\mathbf{G}^{\perp}| \Delta^{\perp}(R_c) \sim \pi.$$

From the behavior $\Delta^{\perp}(R) \sim aR$ we observe^{1]}, one then obtains a peak broadening

$$\delta G \sim \pi/R_c \sim a |\mathbf{G}^{\perp}|.$$

Diffraction peaks in the opposite limit, *i.e.* $|\mathbf{G}^{\parallel}| \gg |\mathbf{G}^{\perp}|$, exhibit systematic departures from linear $|\mathbf{G}^{\perp}|$ peak broadening. The interpolating

form

$$\delta G^2 = |a \mathbf{G}^\perp|^2 + |b \mathbf{G}^\parallel|^2$$

has been fit to experimental data with some success^{7,8} and Horn *et al.*^{7]} have argued that a \mathbf{G}^\parallel term is a consequence of dislocations. If we apply the same argument given above to the rms fluctuations in δx_j , then the corresponding peak broadening takes the form

$$\delta G \sim b |\mathbf{G}^\parallel|$$

where now b comes from the behavior

$$\Delta(R) \sim bR$$

we observe. Therefore, our model, which is *free of dislocations*, reproduces the main features of peak broadening in quasicrystals. Experimentally, the ratio a/b is large.^{8]} Our results, where b depends linearly on δ , give a similarly large ratio suggesting that the analogue of δ in real quasicrystals is also small. Furthermore, we find^{1]} a dependence of strain accumulation on cooling rate, in that slow cooling induces larger strain. This surprising result is consistent with recent experiments in Ga-Mg-Zn.^{9]}

In conclusion, we have studied the dynamic response of different types of 2D elastic networks to homogeneous perturbations. In all the quasiperiodic systems studied, the distortions are bounded, while in the grown samples, the strain accumulation increases linearly with system size. We suggest that the inhomogeneity which causes strain accumulation is a long wavelength modulation in the phason coordinates. We find a dependence of strain accumulation on cooling rate: slow cooling induces larger strain. This striking result is consistent with recent experimental observations.^{9]} Moreover, we propose a mechanism for peak-broadening in quasicrystalline materials which is in sharp contrast with the usual dislocation mechanism.^{7]}

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