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## The relaxation processes of the 2D Penrose pattern: lattice dynamics and electronic structures

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**Abstract.** The vibrational density of states and electronic spectra in the relaxation processes of the 2D Penrose pattern were calculated. The fractal-like spectra due to the self-similarity of the Penrose pattern drastically changed into the continuous spectra without gaps which reflects the FCC(111) crystal structure. At the critical stages defined as the intermediate states between the quasi-crystal and the crystal, the number of localised modes of phonons and electrons increased, indicating the structural transition.

### 1. Introduction

The Penrose pattern, which is widely utilised to understand the quasi-crystal structure, has self-similarity without translational symmetry (Ogawa 1985, Janssen 1986, Janot and Dubois 1988). Consequently, significant features appear in the vibrational and electronic spectra. The electronic structures have mainly been calculated from a theoretical viewpoint (Kohmoto *et al* 1983, Ostlund *et al* 1983). After the discovery of the aperiodic structure by Schechtman *et al* (1984), many papers have been written about the vibrational density of states and/or electronic structures of the 1D Fibonacci chain (Lu *et al* 1986, Liu and Riklund 1987, Nori and Rodriguez 1986, Machida and Fujita 1986a,b, Kohmoto and Banavar 1986, Kohmoto 1986, Kohmoto *et al* 1987, Janssen and Kohmoto 1988, Mookerjee and Singh 1986), the 2D Penrose pattern (Kohmoto and Sutherland 1986a,b, Sutherland 1986a,b, Tsunetsugu *et al* 1986, Odagaki and Nguyen 1986, Kumar and Athithan 1987) and the 3D Penrose pattern (Marcus 1986). The computed spectrum has self-similarity and shows the curves which may be differentiated anywhere, but are continuous. Although the spectra were calculated within the tight-binding approximation, the electronic and lattice dynamic properties peculiar to quasi-crystals were revealed qualitatively. The conductance (Ueda and Tsunetsugu 1987, Choy 1987, Hu and Ting 1986, Mello 1987), plasmons (Sarma *et al* 1986) and electron localisation (Sokoloff 1986, Verges *et al* 1987) of the quasi-periodic structures and the

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electronic spectra of other self-similarity patterns (Nagatani 1985) were also investigated. In our previous letter (Sasajima *et al* 1987), relaxation processes, such as the structural transition from the quasi-crystal (the 2D Penrose pattern) to the normal crystal (the FCC (111) structure), were simulated by the molecular dynamics method. The changes in the phonon and electronic spectra during these processes are of great interest. How do the gaps found everywhere in the spectrum of the Penrose pattern vanish and how does the normal spectrum of the FCC (111) appear? We have computed the vibrational and electronic spectra of the relaxed 2D Penrose patterns by the tight-binding approximation. The localisation of eigenstates was also studied by calculating the participation ratios.

## 2. Methods of calculation

### 2.1. Vibrational density of states

The atomic vibrational frequencies normal to the atomic plane can be given as the solutions of the equations of motion

$$m_i \ddot{z}_i = -\sum_j c^{ij} z_j \quad (1)$$

where  $m_i$  and  $z_i$  are the mass and the displacement, respectively, normal to the atomic plane of the  $i$ th atom and  $c^{ij}$  is the effective coupling constant between the  $i$ th and  $j$ th atoms. Substituting the eigenmode solution,

$$z_i = (u_i/\sqrt{m_i}) \exp(i\omega t) \quad (2)$$

in the equation of motion (1), we get

$$\omega^2 u_i = K_{ij} u_j \quad (3)$$

where

$$K_{ij} \equiv C_{ij}/\sqrt{m_i m_j} \quad (4)$$

is the force constant matrix. The matrix elements (4) were determined from the following two models. Let  $r_{ij}$  be the distance between the  $i$ th and  $j$ th atoms and assume the distance dependence of the matrix elements to be

$$K_{ij} = \exp[-(r_{ij} - 1)] \quad (5)$$

where the distance is measured by the length of the edges of the Penrose tiles. We have considered the following cases: model I is for:

$$0.9 \leq r_{ij} \leq 1.1 \quad (6)$$

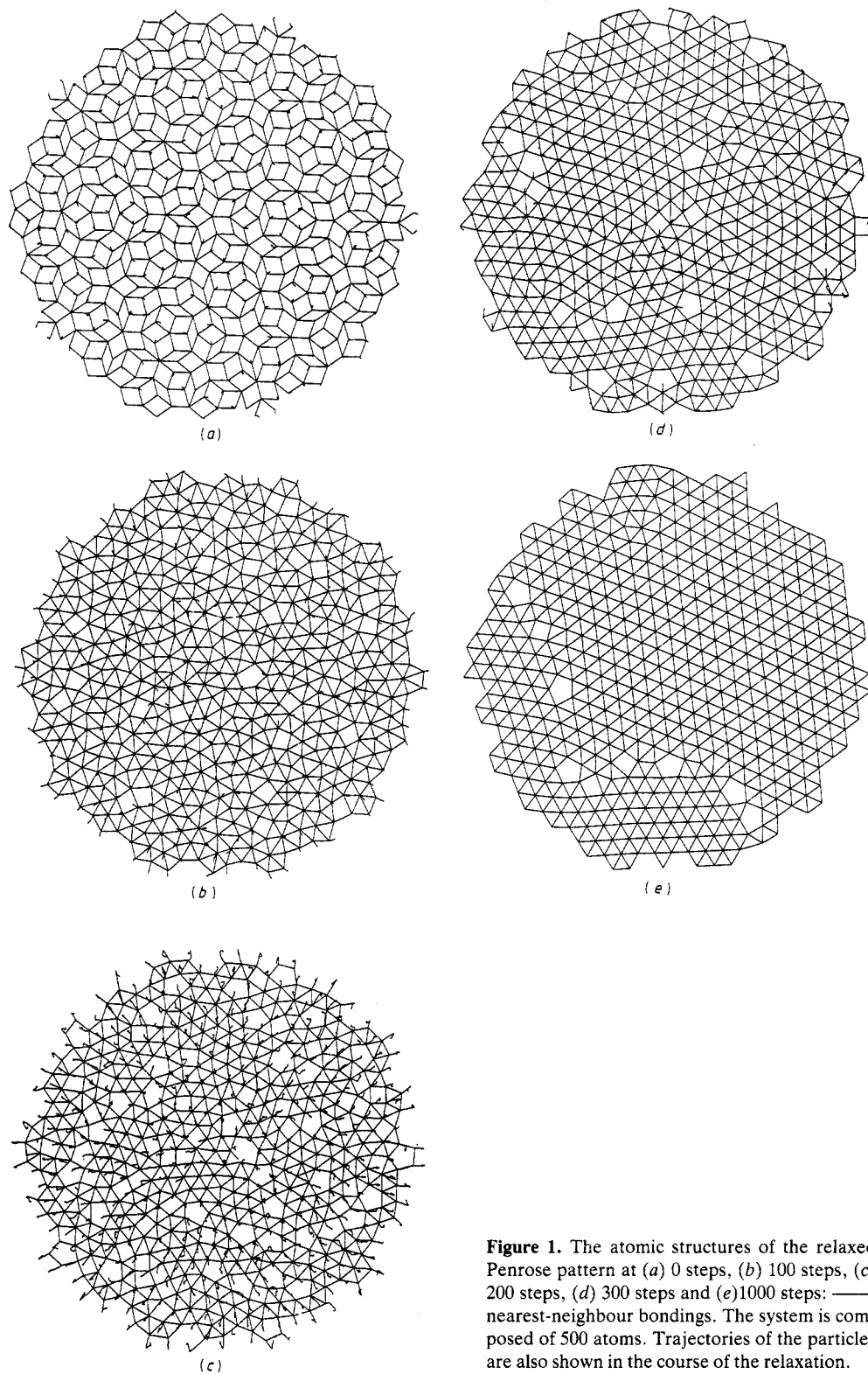
and model II is for

$$r_{ij} \leq 1. \quad (7)$$

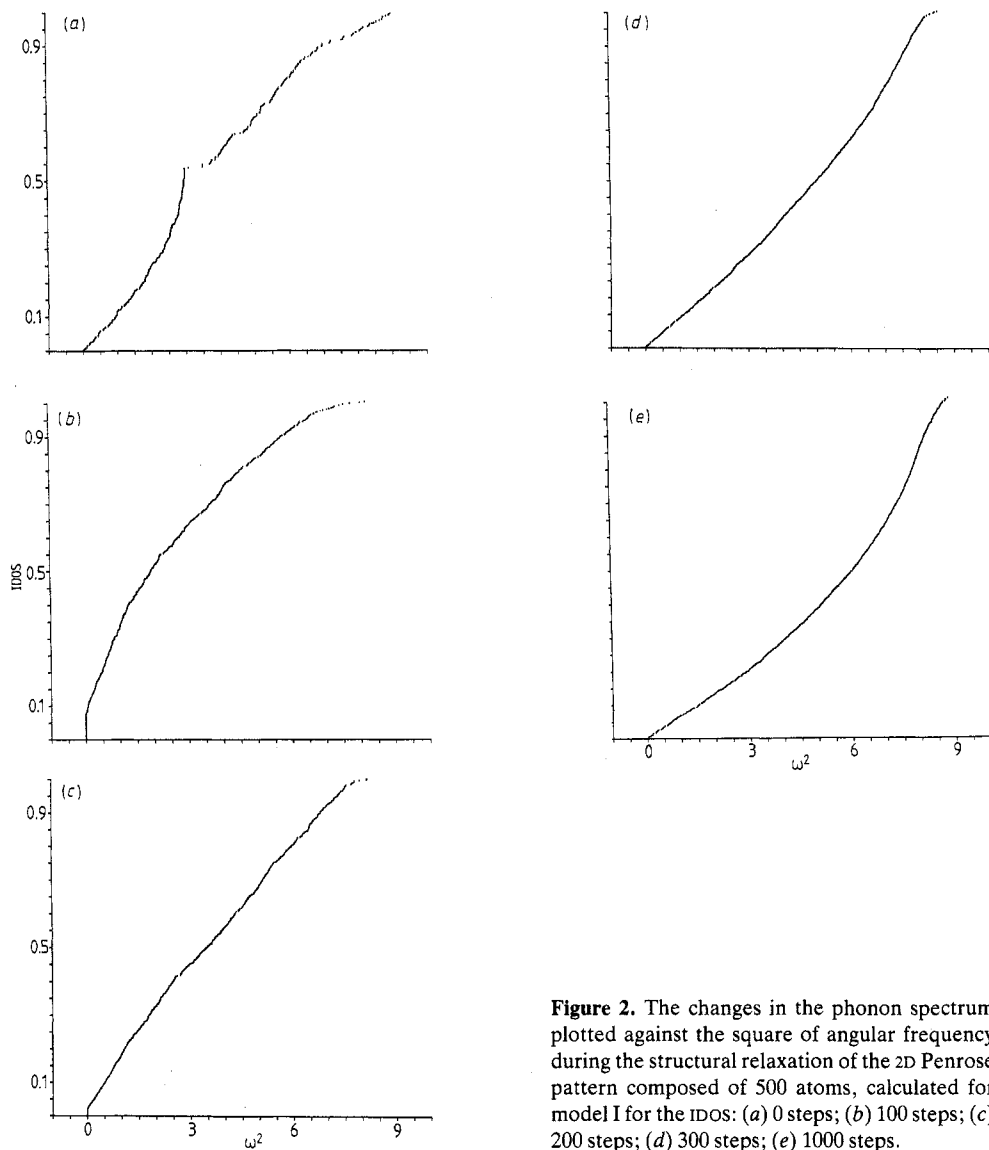
The diagonal elements can be derived from the translational invariance and written as

$$K_{ii} = -\sum_{j(\neq i)} K_{ij} \quad (8)$$

The dynamical matrix was diagonalised to obtain the frequencies and modes of the



**Figure 1.** The atomic structures of the relaxed Penrose pattern at (a) 0 steps, (b) 100 steps, (c) 200 steps, (d) 300 steps and (e) 1000 steps: —, nearest-neighbour bondings. The system is composed of 500 atoms. Trajectories of the particles are also shown in the course of the relaxation.



**Figure 2.** The changes in the phonon spectrum plotted against the square of angular frequency during the structural relaxation of the 2D Penrose pattern composed of 500 atoms, calculated for model I for the IDOS: (a) 0 steps; (b) 100 steps; (c) 200 steps; (d) 300 steps; (e) 1000 steps.

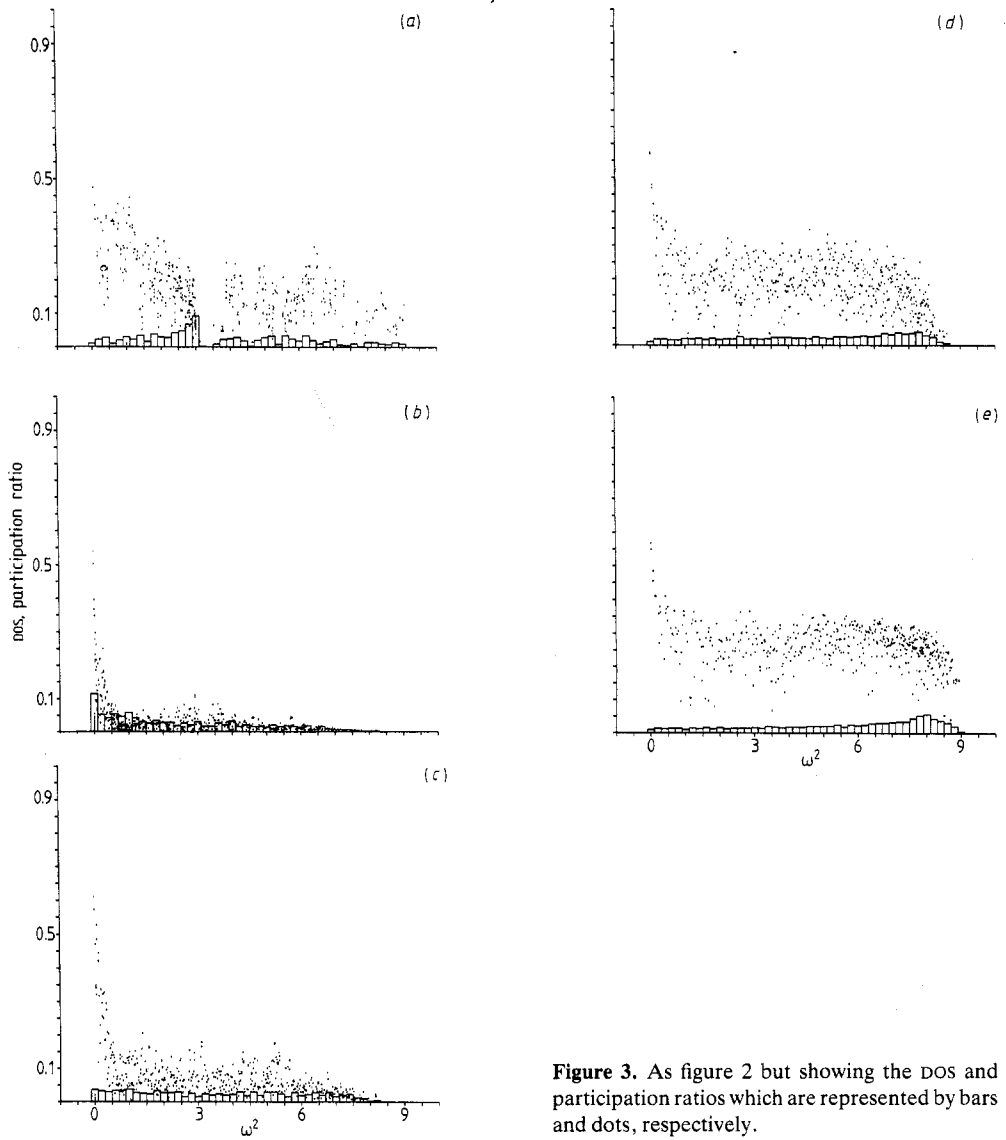
vibrational eigenstates. Model I selects only the networks of the sides of the Penrose tiles and model II expresses the central-force approximation or spherical symmetry of the *s*-like orbitals in the electronic structure.

## 2.2 Electronic spectrum

We assumed the following tight-binding Hamiltonian of *s*-type orbitals:

$$H_{ij} \equiv \langle i | H | j \rangle \quad (9)$$

where  $|i\rangle$  denotes the *s*-type orbital of the *i*th atom and *H* is the effective one-electron Hamiltonian. Similar to models I and II, non-zero matrix elements were obtained as



**Figure 3.** As figure 2 but showing the DOS and participation ratios which are represented by bars and dots, respectively.

$$\langle i | H | j \rangle = -\exp[-(r_{ij} - 1)] \quad (10)$$

where the diagonal elements were chosen as zero in order to make the energy of the isolated orbital zero:

$$\langle i | H | i \rangle = 0. \quad (11)$$

### 2.3. Participation ratio

If we write the  $\mu$ th eigenstate of the Hamiltonian as

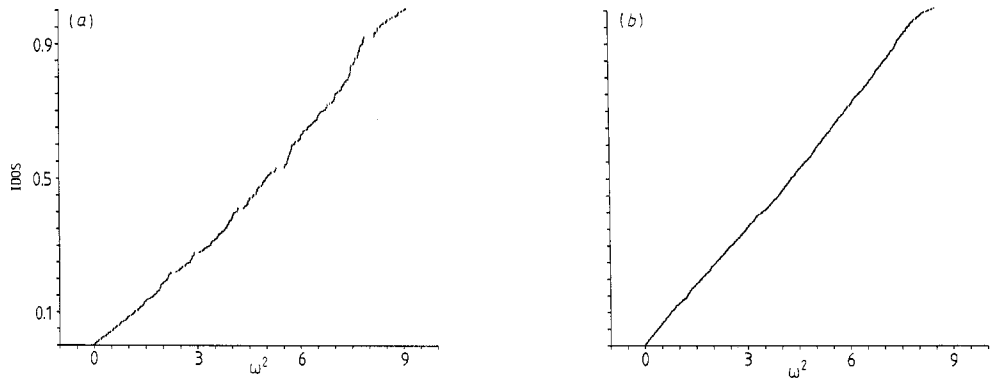


Figure 4. Similar to figure 2 but using model II: (a), 0 steps; (b), 100 steps.

$$|\mu\rangle = \sum_i a_i^\mu |i\rangle \quad (12)$$

the participation ratio (Odagaki and Nguyen 1986) is defined as

$$P_\mu = \sum_i |a_i^\mu|^2 / N \sum_i |a_i^\mu|^4 \quad (13)$$

where  $N$  is the total number of atoms.  $P_\mu$  varies from  $1/N$  to 1:  $P_\mu = 1/N$  means that the electron at the  $\mu$ th eigenstate localises on an atomic site;  $P_\mu = 1$  means that the  $\mu$ th eigenstate is an extended state and the wavefunction of the electron is uniformly distributed over the whole system. This parameter represents the degree of localisation and can also be applied to the atomic vibrational states.

### 3. Results and discussion

The vibrational spectra and the electronic spectra for the systems of 76 and 500 atoms were calculated. The computed results are shown only for the 500-atom case. Results

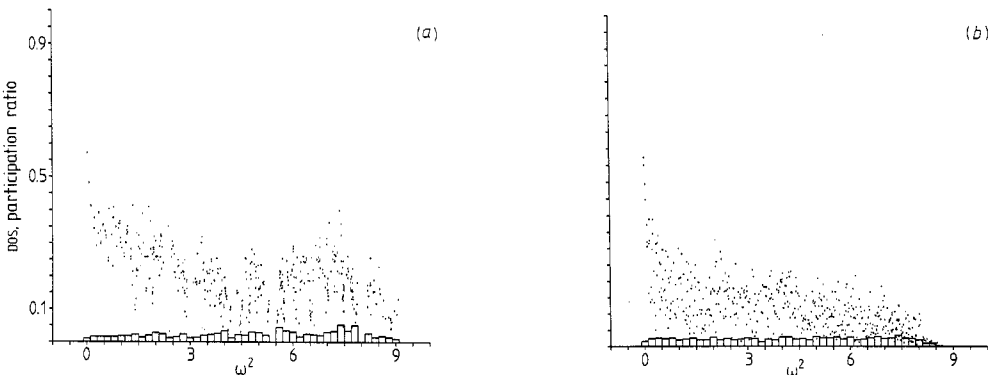
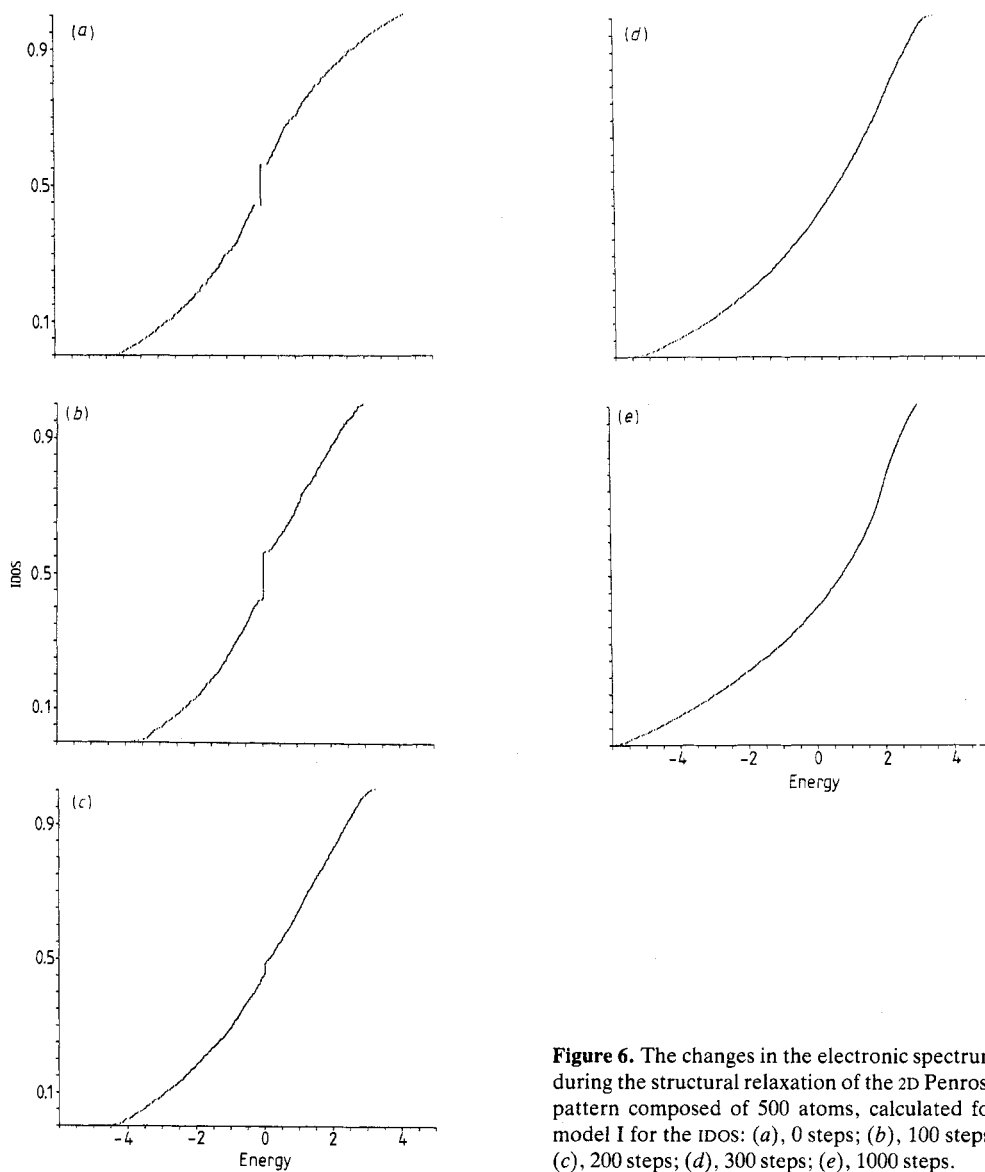


Figure 5. Similar to figure 3 but using model II: (a), 0 steps; (b), 100 steps.

for the larger systems containing 1000, 1500 and 2000 atoms are similar to those containing 500 atoms. To aid discussion, the structures of the calculated 500 atoms at 0, 100, 200, 300 and 1000 steps are shown in figure 1. The relaxation time step is of the order of  $10^{-15}$  s.

### 3.1. Phonon spectrum

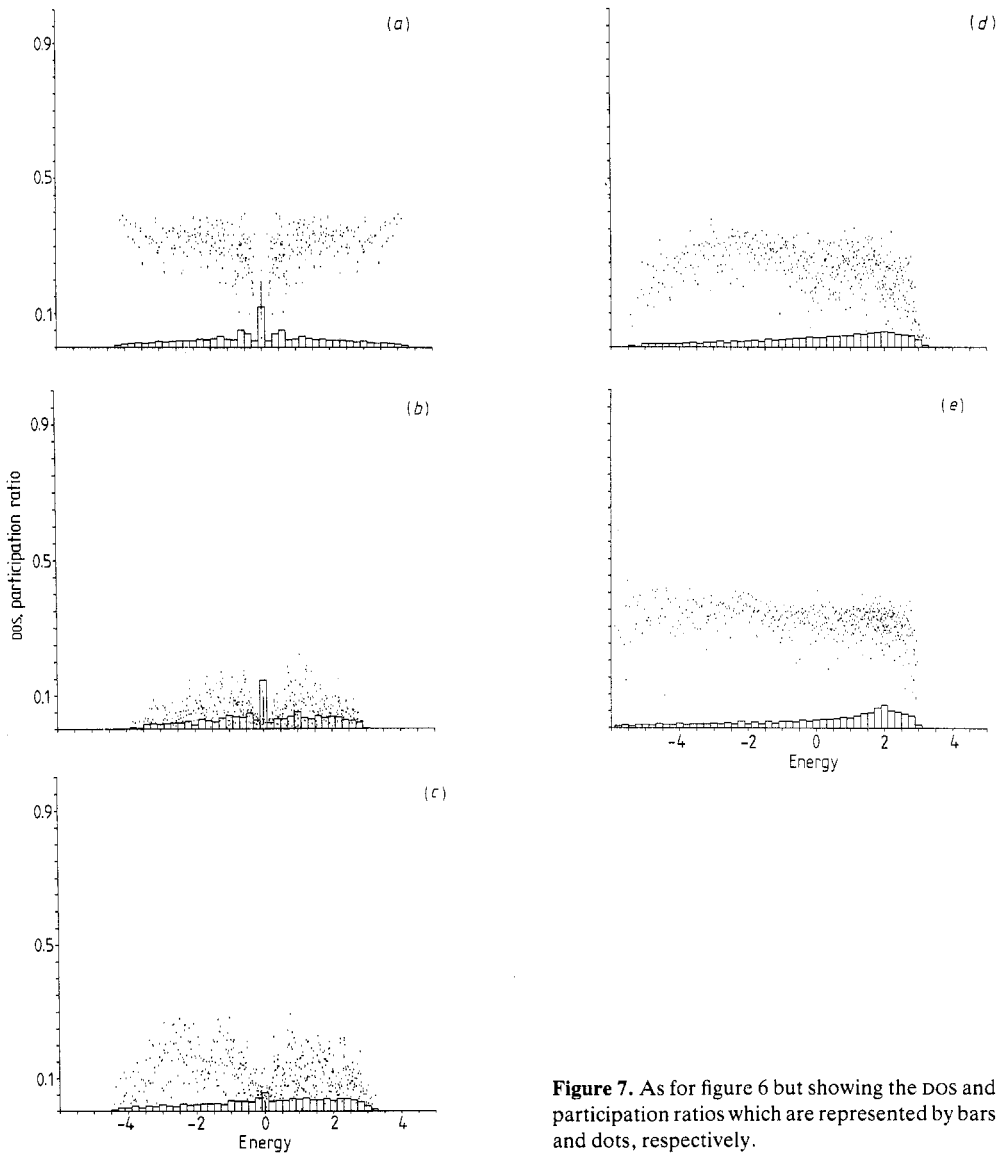
Figure 2 shows the integrated density of states (IDOS) and figure 3 the density of states (DOS), respectively, with participation ratios which were calculated using model I. As



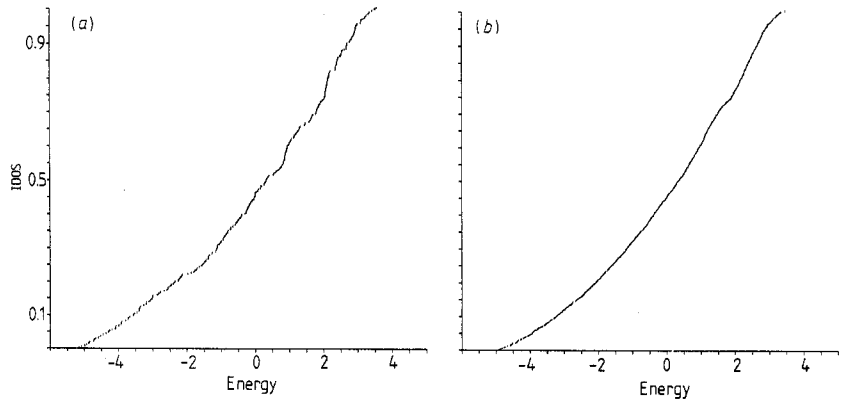
**Figure 6.** The changes in the electronic spectrum during the structural relaxation of the 2D Penrose pattern composed of 500 atoms, calculated for model I for the IDOS: (a), 0 steps; (b), 100 steps; (c), 200 steps; (d), 300 steps; (e), 1000 steps.



can be seen, fractal-like gaps disappeared between 200 and 300 steps, which corresponds to the structural transition from the quasi-crystal to the crystal structures. The critical states of the transition appeared at 100 steps and show a drastic lowering of the participation ratios and an increase in the soft-phonon modes. In the crystal phase the IDOS should be proportional to  $\omega^2$  in the  $\omega \rightarrow 0$  limit because of the 2D continuous-medium approximation. For model II, the results at 0 and 100 steps are shown in figures 4 and 5. We could not find any drastic change in the participation ratios or phonon softening in this model. This is probably due to the additional bondings which do not exist in model I. Other characteristic features of the changes in the spectra were similar to those of model I.



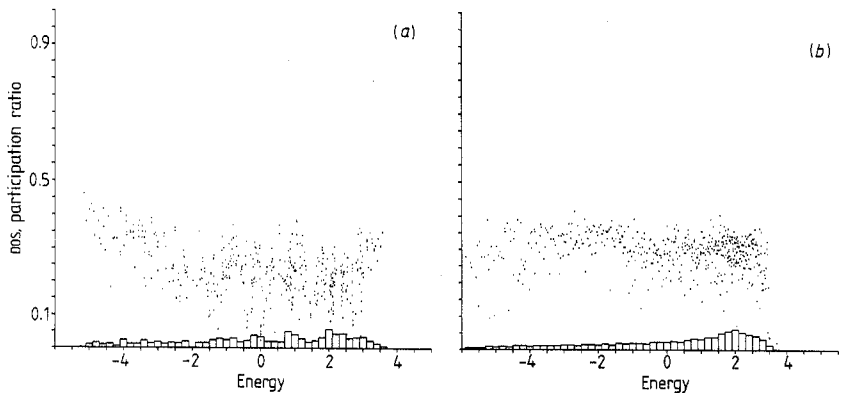
**Figure 7.** As for figure 6 but showing the DOS and participation ratios which are represented by bars and dots, respectively.



**Figure 8.** Similar to figure 6 but using model II: (a), 0 steps; (b), 100 steps.

### 3.2. Electronic spectrum

Figure 6 shows the IDOS and figure 7 the DOS, respectively, with participation ratios calculated using model I. The spectrum of the Penrose pattern (0 steps) shows fractal-like gaps, 7% degeneracy at zero level and inversion symmetry about the band centre. These exotic features are well known to be caused by self-similarity of this pattern. It should be noted here that zero-level degeneracy and symmetry of the spectrum are distinct if other bondings are included such as in model II (figures 8(a) and 9(a)). The changes in the spectrum were completed at 300 steps, which corresponds to the end point of the structural transition, as already mentioned above. At 100 steps, which is considered to be the transition stage of the structure, the number of zero-level states increased and participation ratios for all states drastically decreased. After these transition stages, the spectrum shows continuous curves, and the continuous-medium approximation holds fairly well. For model II, computed results show similar trends to those of model I but some significant features such as the lowering of participation ratios and an increase in the zero-level modes are not evident. We show the results at 0 and 100 steps in figures 8 and 9.



**Figure 9.** Similar to figure 7 but using model II: (a), 0 steps; (b), 100 steps.

#### 4. Conclusions

The changes in the phonon and electronic spectra for the structural transition from the quasi-crystal to the crystal phases were studied. Two kinds of model were examined for the calculation; the networks of the Penrose tiles were considered in model I and the spherical symmetry of the bondings was assumed in model II. Both models showed completion of the structural changes at 300 steps. The continuous spectrum reflecting the periodicity of crystals appeared instead of fractal-like gaps caused by the quasi-periodic structures. Model I showed the following extra characteristic features at the structural transition.

(i) The participation ratios drastically decreased in both vibrational and electronic spectra.

(ii) Phonon softening and increase in the zero-level states were found for vibrational and electronic states.

In this paper, the calculation was performed only for the monatomic case but these methods can be easily adapted to two-atom systems. The stability of the more realistic models of quasi-crystal structures such as those of Socolar and Steinhardt (1986) and Henley (1986) will be reported in the near future.

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