

BREATHERS AND KINKS IN A SIMULATED CRYSTAL EXPERIMENT

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ABSTRACT. We develop a simple 1D model for the scattering of an incoming particle hitting the surface of mica crystal, the transmission of energy through the crystal by a localized mode, and the ejection of atom(s) at the incident or distant face. This is the first attempt to model the experiment described in Russell and Eilbeck in 2007 (EPL, **78**, 10004). Although very basic, the model shows many interesting features, for example a complicated energy dependent transition between breather modes and a kink mode, and multiple ejections at both incoming and distant surfaces. In addition, the effect of a heavier surface layer is modelled, which can lead to internal reflections of breathers or kinks at the crystal surface.

1. Localized modes in Mica. We describe elsewhere in these proceedings [8] the central puzzle (what cause most of the macroscopic tracks in mica crystals) and our interpretation (that these tracks are caused by quasi-particles called quodons, which we postulate are longitudinal breathers). In particular, in this paper, we concentrate on the experiment described in [7]. In that paper, we describe a scattering experiment, where alpha particles impinging on a mica crystal generate ejected particles from the opposite face of the crystal. Since the crystal in question is of dimension of about 10^7 lattice units, some quasi-particle must have traversed this distance carrying sufficient energy to eject an atom. We call this quasi-particle a *quodon*, and postulate that it is a localized vibrational mode or breather.

In order to test this hypothesis, it is necessary to model the experimental setup and obtain agreement between theory and experiments. It is believed that the K sheet in mica is responsible for supporting such a breather, as the other planes are too rigid. Our first step in this direction was a 2D simulation of breathers in a

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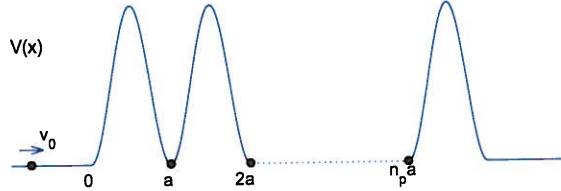


FIGURE 1. Idealised model finite sized 1D mica crystal. Note an incoming particle on the left about to strike the face of the crystal.

hexagonal lattice representing the K sheet [6]. We found evidence for mobile longitudinal optical breathers which traversed about 10^4 lattice units before breaking up. Some recent studies by Yi et al. [9] have shown similar results in a somewhat different lattice model. If quodons are indeed breathers, we still have a large factor of 10^3 or more to account for in the comparison between 2D models and the actual mica experiments and observations. It may be that our model is insufficiently detailed or missing some important feature, for example longer range interactions rather than the nearest neighbour interactions assumed in the calculations. It may be that the full 3D case would introduce some new features which would increase the breather lifetimes. We plan to return to this problem in the near future.

The calculations in [6] were also limited with respect to modelling the experimental situation in [7], as no surface effects were considered. Our plan in this paper is to present a modest 1D toy model which includes surface effects and hence is the first step in modelling the recent experiments. In all other respects the model is a step backward, as it considers only 1D effects and looks only at acoustic breathers (i.e. breathers with in-phase oscillations). Nevertheless it throws up some interesting new features which may be of interest. In particular, as the energy of the incoming particle increases, there is a transition in the internal localized mode created, between a breather mode and a kink mode. However this transition is complicated by a third intermediate situation, where a very slow or stationary breather is created, apparently pinned by the lattice. Depending on the energy of the internal mode, multiple ejections at both incoming and distant surfaces are possible. In addition, the effect of a heavier surface layer is modelled, which can lead to internal reflections of breathers or kinks at the crystal surface.

The paper is set out as follows. We describe the model in the next section, and Section 3 we briefly describe the results of various simulations at increasing values of the energy of the incoming particle. In Section 4 we consider the interesting case where the boundary particle(s) have a higher mass than those in the rest of the crystal. Finally some conclusions are given in Section 5.

2. The model. Our idealised 1D model for the mica crystal experiment [7] is shown in Fig 1. In the model, each atom in the crystal sits inside a harmonic lattice potential, which is meant to model the effects of the adjacent sheets in a higher dimensional crystal. Outside the surface the potential is set to be zero. Note an incoming particle with velocity v_0 about to strike the surface. Particles are free to be ejected into the vacuum on either side, from either the incident face or the distant face, subject to the forces acting on them. We assume all atoms inside the crystal are at rest at a local minimum of a potential, i.e. at absolute zero with no

temperature effects. Our Hamiltonian is thus

$$H = \sum_{i=0}^{n_p} \left[\frac{1}{2} \dot{x}_i^2 + V(x_i) + W(x_i - x_{i-1}) \right],$$

where the on-site potential V is

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \text{ or } x > L, \\ \frac{a^2}{4\pi^2} (1 - \cos(\frac{2\pi x}{a})) & \text{otherwise.} \end{cases}$$

In addition, the atoms are assumed to interact through an inter-particle force given by a nearest neighbour Morse potential $W(x_i - x_{i-1})$, where

$$W(x) = \frac{1}{2b^2} [\exp(-b(x-a)) - 1]^2.$$

Note the minimum of the Morse potential is assumed to coincide with the lattice spacing a . However no correction is made at the surface for the absence of a second particle to balance these forces, so our model starts off unrelaxed with some small residual energy at the end points.

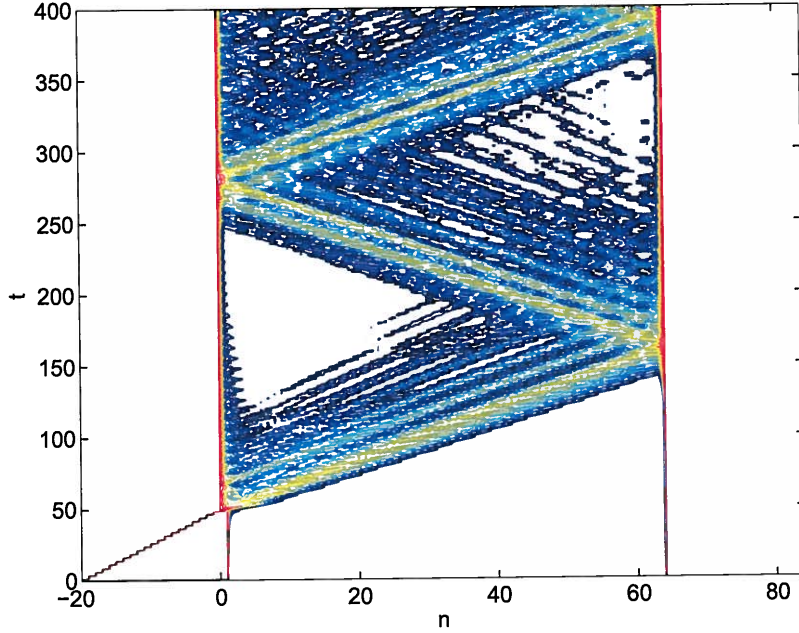
As a further simplifying assumption, we assume the incoming particle has the same (unit) mass and inter-particle force as the atoms resident in the crystal. We have modelled the surface potential in the simplest way possible, by merely truncating the harmonic lattice potential to zero at each end at the value corresponding to the minimum of the sinusoidal potential. Some alternative simulations with the external constant potential corresponding to the maximum of the sinusoidal potential have also been tried: in general the quantitative behaviour in this case is very similar.

For simplicity we consider a small lattice of $n_p = 64$ stationary particles, plus one incoming particle. In all our simulations we set $a = 1$ and $b = 2$. Except in the final section, all the masses in the problem are normalized to unity. The initial conditions are that particles $1, \dots, n$ are at rest at $x_i = ia$, and particle 0 is incoming at $-20a$ with velocity v . The left hand boundary of the crystal is at $x = 0$ and the right hand boundary is at $x = L \equiv (n_p + 1)a$. In order for H to be defined for all $i = 0, 1, \dots, n_p$, we introduce two fixed particles -1 and $n_p + 1$ at $x = -1000a$ and $x = 1000a$ respectively.

An analysis of the linearised system shows that low amplitude coupled oscillators with frequency below the phonon band must oscillate in phase [4, 5], so we do not expect optical breathers in this system. We refer the reader also to some previous studies of this system, in which the interaction of breathers with both vacancies and with interstitial defects [1, 2, 3].

3. Dynamic simulations. In this section we report a preliminary study with the model described above, varying a single parameter, the velocity of the incoming particle v_0 .

3.1. $v_0 = 0.4$. For low values of v_0 , the incoming particle generates a low amplitude fast acoustic breather which is reflected by the boundaries but eventually begins to spread out and disperse. Fig 2 shows an example for $v_0 = 0.4$. At these energies the displacement of the atoms in the lattice does not show up clearly without some artificial scaling, so we have chosen to display instead a contour plot of the local energy density. Note that in this figure and all subsequent energy plots, we are taking contours of the logarithm of the energy. This has the effect of picking out small background effects, which might otherwise be swamped by the main localized

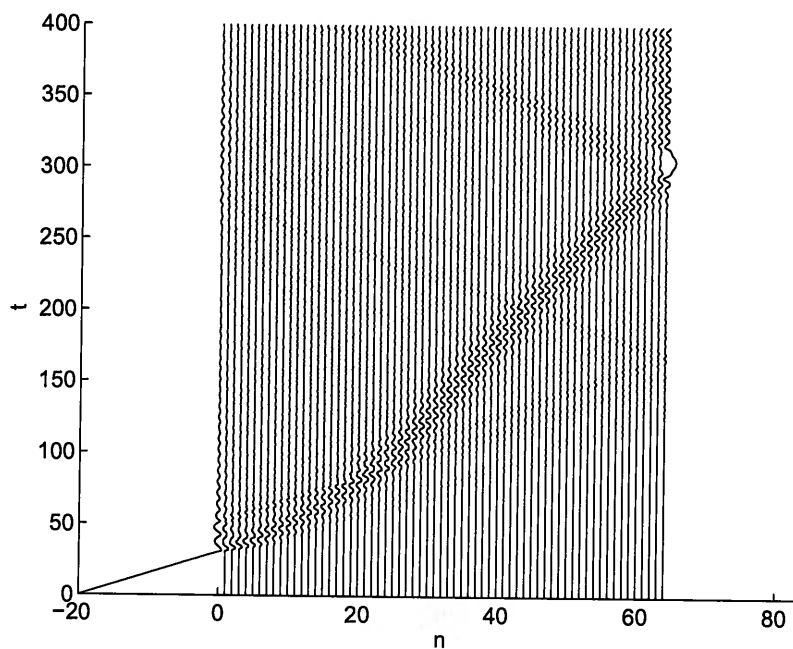
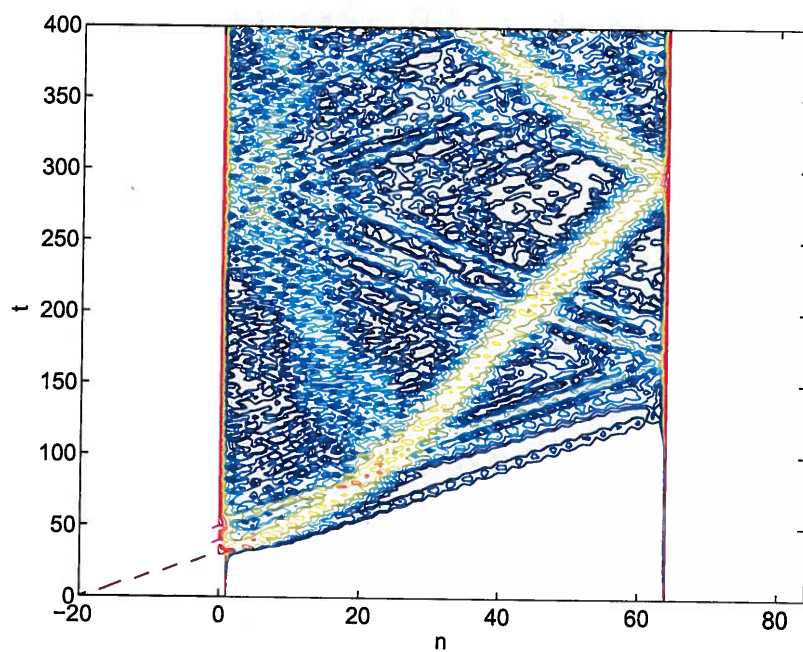
FIGURE 2. Energy contours, $v_0 = 0.4$

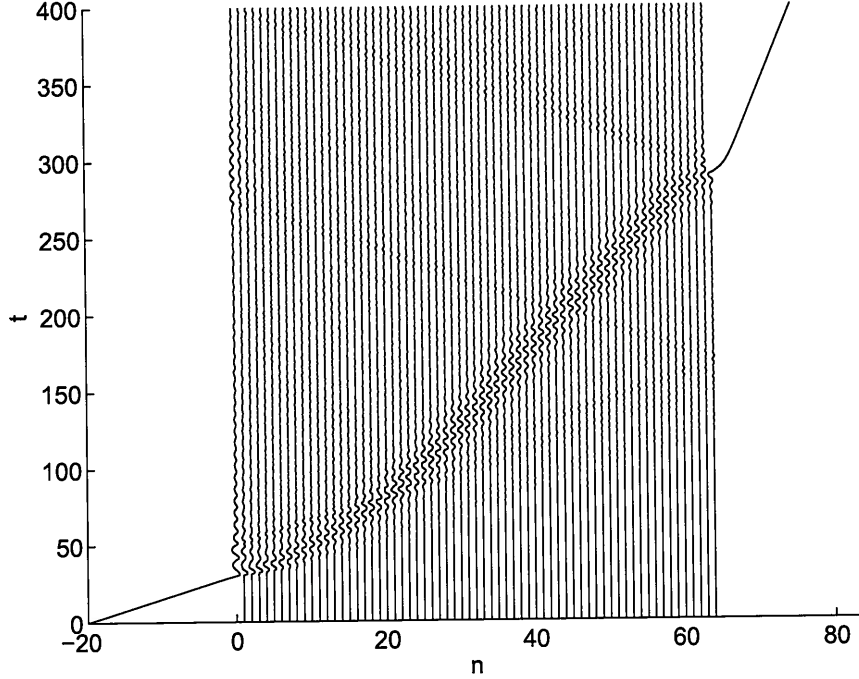
mode moving through the system. We see a small border region of high energy on each side due to the unrelaxed boundary conditions.

3.2. $v_0 = 0.65$. As we increase v_0 further, the breather induced by the incoming collision becomes slower and more energetic. When it reaches the back face of the crystal, the breather sometimes has sufficient energy and a suitable phase to eject a particle. The combination of energy and phase is crucial, the final particle in the system will undergo a strong induced oscillation, but this oscillation must be in phase with the rest of the breather to accumulate enough energy for ejection. Due to this effect we find a number of windows in the v_0 space giving ejection, with other regions showing no effects except the internal reflection of the breather at the surface.

A typical example of the “reflection only” mode is shown in Fig 3. Here we have chosen to display the particle trajectories as a function of time for the case $v_0 = 0.65$. The slanting line on the left shows the incoming particle, which excites a mobile breather which then travels to the right. The incoming particle sticks to the surface, held there by the inter-particle force between it and the first atom in the crystal. Some of the energy is reflected in a smaller breather, and the rest remains the back face, with the right-most atom making a small excursion into the void on the right, but without enough energy to escape completely.

The corresponding contour plot of the local energy density in this case is shown in Fig 4, with the same parameters as Fig 3. The main breather moving through the system can be clearly seen, as in Fig 3. However this plot shows some interesting fine detail which is not clearly revealed in 3. A number of small localized high

FIGURE 3. Particle trajectories, $v_0 = 0.65$ FIGURE 4. Energy contours, $v_0 = 0.65$

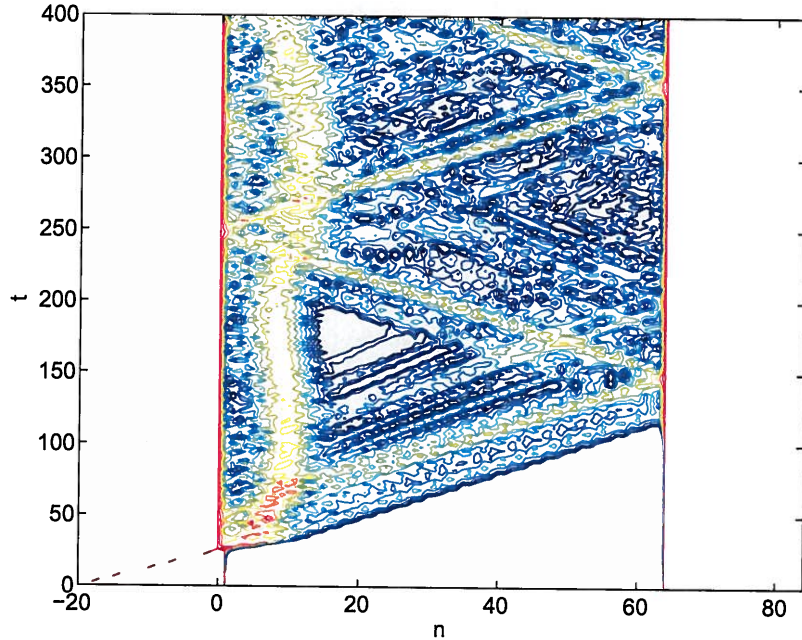
FIGURE 5. Particle trajectories, $v_0 = 0.66$

speed modes are shown, together with a more extended mode which breaks off from the main breather and travels slowly to the left before colliding with the boundary and sticking loosely in this position. It would be interesting to study these modes further.

A further possibility, which we plan to investigate, is to fire a sequence of atoms at the crystal. As the energy builds up on the back face, this will make it easier for subsequent breathers to eject atoms from this “hot-spot” site.

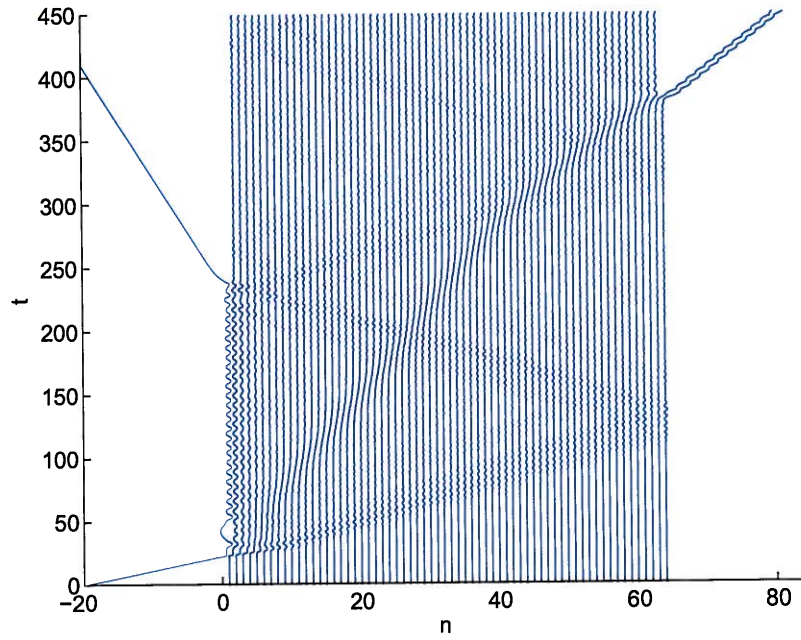
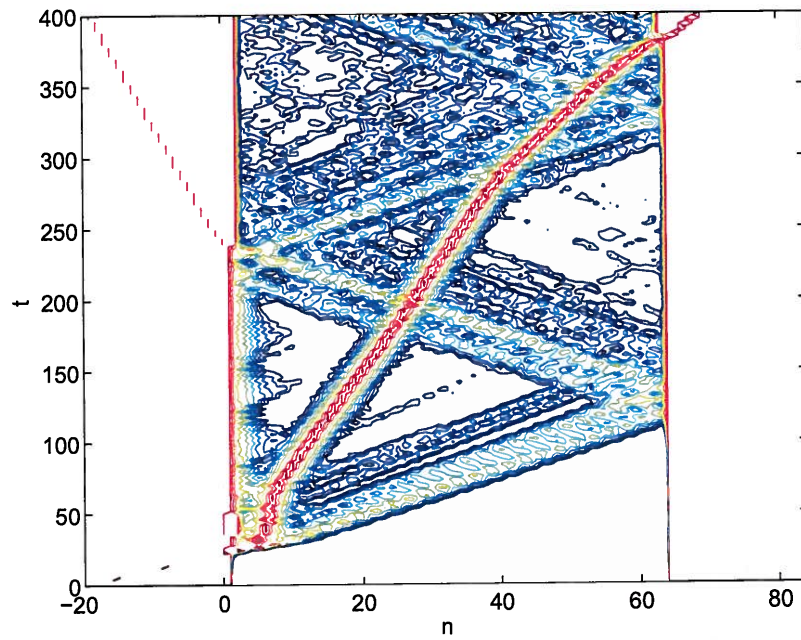
3.3. $v_0 = 0.66$. If we increase v_0 slightly from 0.65 to 0.66, we enter a “ejection window” and get the trajectory plot shown in Fig 5. Although the creation and transmission of a breather proceeds as before, when it reached the right-hand boundary, a particle is ejected. We emphasize again that this is not just because an energy threshold for ejection has been reached, but because also the *phase* of the breather is favourable when the boundary is reached. If for example the length of the crystal is increased slightly, the phase of the breather may be different when it reached the boundary, and no ejection is observed. So it is not possible to predict whether or not ejection takes place from knowledge of v_0 alone. It would be interesting to examine a detailed range of v_0 in this region to chart the different windows – we have observed at least three, but there may be many more.

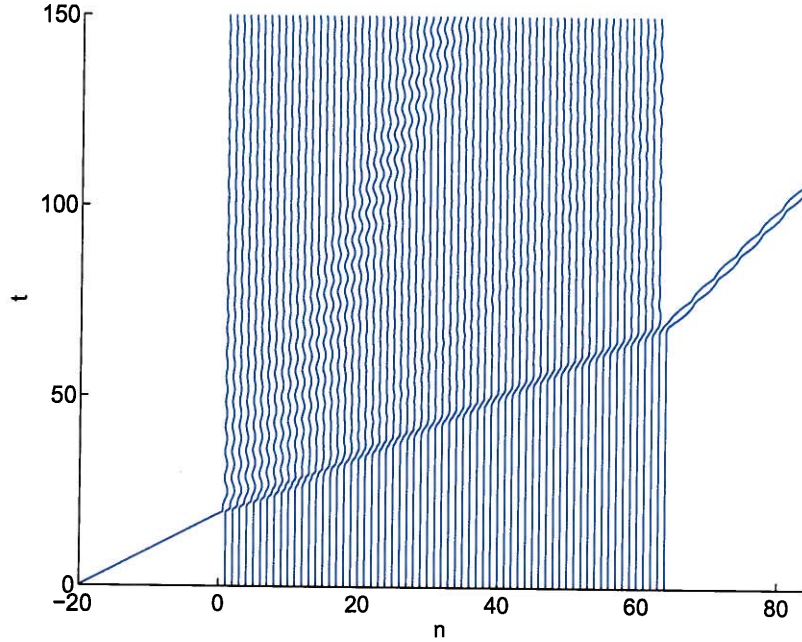
3.4. $v_0 = 0.8$. Naively one might think that if we continue to increase the value of v_0 , the energy of the induced breather is increased accordingly, and ejection is more likely at the far edge of the crystal. However it has long been observed that at

FIGURE 6. Energy density plot, $v_0 = 0.8$

higher energies, the discreteness of the lattice plays an increasingly important role in breather propagation, and eventually we get a “pinning” effect. In the current model this is indeed observed. The effect is most easily seen with an energy contour plot. If we increase v_0 to 0.8, we get the result shown in Fig 6. When the incident particle hits the crystal, a stationary localized mode is formed which after a delay throws off some small high-speed breathers. The bulk of the energy stays trapped close to the l.h. boundary, although some small oscillations in its position are seen. However we have again observed sensitive behaviour dependent on initial conditions - for a small change in v_0 the velocity and trajectory of the induced breather can be quite different.

3.5. $v_0 = 0.88 - 0.89$. As v_0 increases further, we enter a complicated region with results even more sensitive to the specific value of v_0 used. We get the first examples of kinks occurring simultaneously with mobile breathers, also stationary surface breathers at the incident surface which can lead to ejections from this face. A nice example showing all three effects together is shown below in Fig 7 for $v_0 = 0.887$, which should be studied in conjunction with the corresponding energy density plot in Fig 8. In this example the incoming particle interacts in a complicated way with the atoms in the incident surface. A boundary excitation is set up which persists for a long time. Meanwhile a small fast breather is generated which travels to the far edge and is reflected. When it returns to the incident surface, it has sufficient energy to nudge the surface mode into ejecting an atom to the left. Note that if our model included internal vacancies or interstitials, we would expect that in at least some cases the mobile breather would be reflected by this impurity, and

FIGURE 7. Particle trajectories, $v_0 = 0.887$ FIGURE 8. Energy density plot, $v_0 = 0.887$

FIGURE 9. Particle trajectories, $v_0 = 1.05$

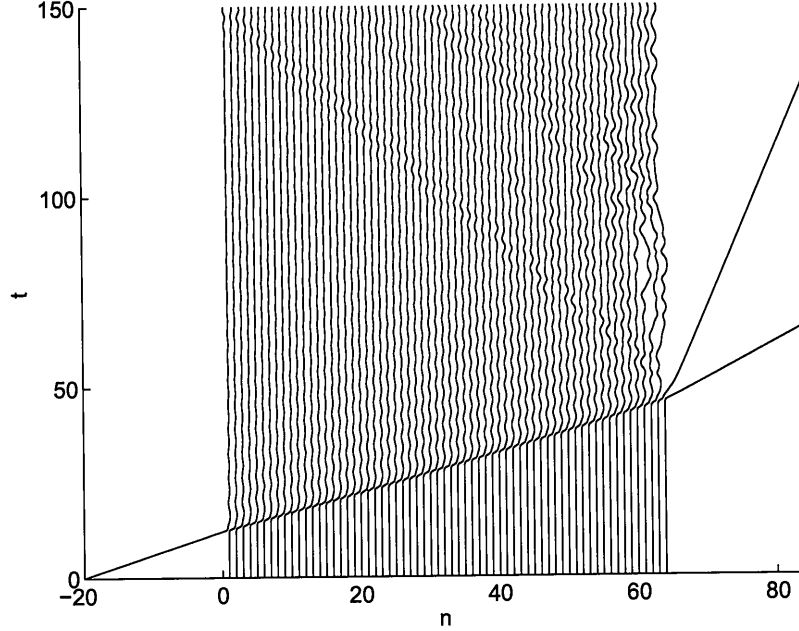
a similar effect might be induced. In sputtering experiments a delayed ejection of this sort has often been seen, in specific crystal axis directions, but the suggested mechanism is very different.

In addition to all this a travelling topological kink is formed which moves more slowly from left to right, and ejects two particles at the right-hand face. By kink we mean a local mode in which the atom in a particular potential well suffers a permanent translation to the right or left as the mode travels through.

Other choices of v_0 in the range $v_0 = 0.88 - 0.89$ gives a variety of combinations of phenomena, including immediate ejection of atoms from the incident face, formation of vacancies just inside the incident face, single or double ejections from the far face, etc.

3.6. $v_0 = 1.05$. If we further increase v_0 to 1.05, the trapping phenomena switches to pure kink behaviour, with no significant breather activity. This is illustrated in Fig 9. Now the incoming particle induces a more energetic topological kink. There is little evidence of a faster breather, as in Figs 7, 8. When the kink reaches the right-hand boundary, as in the previous case, it has sufficient energy to eject two particles, which stay close enough together to be bound by the inter-particle potential. In addition some energy is deposited in a breather close to the left hand boundary, where it moves slowly to the right in contrast to the one shown in Fig 6.

3.7. $v_0 = 1.65$. A further increase in v_0 does not apparently produce any new internal localized mode, it seems always the case that kink is formed, although the higher the energy, the narrower the kink appears. Fig 10 shows a calculation with $v_0 = 1.65$. The main qualitative difference with the previous diagram is that in this

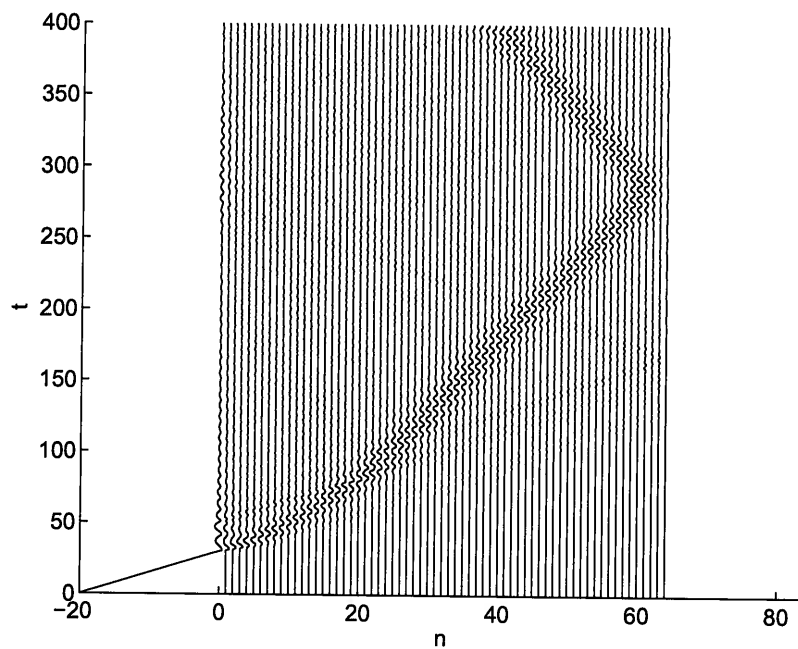
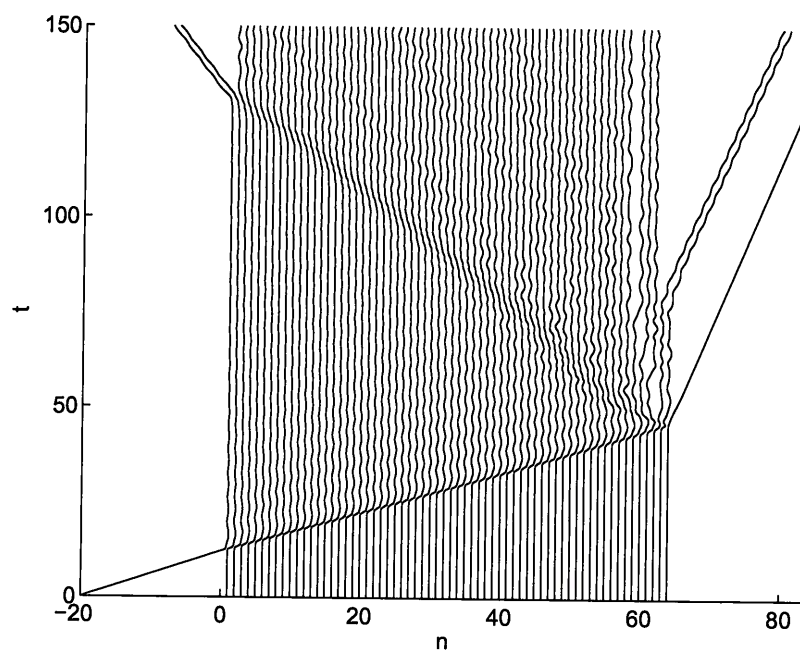
FIGURE 10. Particle trajectories, $v_0 = 1.65$

case the two ejected particles are no longer bound together but are thrown off with two different velocities. In addition, a lot of energy is left at the boundary after ejection, some of which is reflected as one or more breathers.

4. Higher mass boundary layers. In some applications [8], we may wish to reduce the possibility of ejection and increase the amount of energy that undergoes internal reflection at a boundary. This could enable us to have a much longer breather lifetime in a small crystal. A good approximation to fixed rigid boundary conditions is to increase the mass of one or more of the boundary atoms in the crystal. This could be effected in practice by depositing a layer of heavy atoms on the surface by sputtering. The effect of having a single atom on the right hand boundary, with 10 times the mass of the other atoms in the crystal, is shown in Fig 11 for the case $v_0 = 0.66$. This should be compared with Fig 5 for the single mass case. It is clear that ejection is suppressed and more energy is reflected. In view of the sensitivity of the ejection process to phase, etc., we should report that this feature seems robust in several test runs with similar parameters.

This situation would also model approximately the case of a heavy impurity at an internal site in the crystal, if impact energies were low.

However, once we go to high energies, we can get very different and more complicated features. Fig 12 shows this for the case $v_0 = 1.65$. This should be compared with Fig 10 for the single mass case, and also Figs 7, 8. Now there is an initial ejection at the r.h. face when the initial kink hits, but some of the energy is reflected in a slower kink which in turn ejects two particles from the r.h. face when it arrives. Meanwhile much energy is left in a complicated stationary mode at the r.h. face.

FIGURE 11. Particle trajectories, $v_0 = 0.66$, r.h. mass 10 unitsFIGURE 12. Particle trajectories, $v_0 = 1.65$, r.h. mass 10 units

Some of this results in a reflection of a less energetic kink which in turn ejects two particles from the l.h. face when it arrives. The remaining energy pinned at the r.h. face eventually ejects two more particles after a delay, leaving an embedded vacancy (stationary anti-kink). In contrast to Figs 7, 8, these high energy effects are qualitatively more robust to small changes of v_0 . Note that the ejection at the l.h. face can be considered as a delayed sputtering, and could equally well be caused by reflection from an embedded impurity in the crystal. We have already remarked on the delayed sputtering phenomena in our discussion of Figs 7, 8.

5. Conclusions. Our preliminary study shows that we can induce acoustic (in phase) breathers by scattering and these can eject atoms in some cases. As the energy of the incoming particle increases, there seems to be a transition from mobile breathers to trapped breathers, then a further transition from trapped breathers to mobile kink as energies increase. These transitions are complicated by the fact that particle ejection and other phenomena depend on the phase of the induced breathers as well as their amplitudes. In addition there is very sensitive response to initial conditions due to the various nonlinear resonances in the system. We further show that heavy atom(s) at boundaries can simulate fixed boundary conditions and increase reflection of energy. Our work has thrown up a number of interesting effects deserving more systematic study in the future. For example we need to map out in detail the different phenomenon ranges, and the properties of generated kinks and breathers after the initial impact and after collisions with distant boundaries. The development of the initial motions on impact also requires further investigation. The effect of a sequence of incident particles rather than just one is also worth studying.

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