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The power spectrum associated with a kink chain oscillating in a non-stokesian atmosphere of paraelastic interstitials

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Abstract

The power spectrum of a built-in kink chain oscillating in an atmosphere of paraelastic interstitials was investigated numerically using a fast Fourier transform technique. Above a sharply defined value of the strain amplitude, odd-harmonic generation is observed only at the low-temperature side of the dislocation relaxation peak associated with interstitial–kink interaction. At moderately high strain amplitudes, a strong enhancement of the harmonics situated in the immediate vicinity of the natural resonance frequency of the chain and complete depression of the rest are clearly seen. Finally, the onset of quasi-chaotic kink oscillations is detected when the system is driven into the super-Snoek regime where atmospheric tearing takes place.

1. Introduction

The investigation of the forced vibrational properties of non-linear systems is of great importance in numerous solid state physics problems. In the context of heat conductivity, thermal expansion, lattice dynamics, impurity modes and non-linear optics [1], it has led to the development of perturbation techniques that have been successful in explaining experimental results. These cases all deal with non-linearity in the potential energy [2] term (anharmonicity) in the equation of motion which may display a set of cascading bifurcations into a chaotic state. In a previous paper [3], we studied the non-linear Debye-type damping (drag) behaviour of an isolated single kink in an atmosphere that displays hyposonic and hypersonic viscosity regimes, in the presence of high external periodic fields (simple harmonic). The computer simulations in this system showed the existence of dissipative resonance behaviour with zero Q^{-1} factor and the occurrence of unusually sharp (quasi-quantum jumps) energy dissipations, similar to Cherenkov radiation, when the kink velocity exceeds the atomic hopping velocity of interstitials at high driving force amplitudes. In the present investigation, we use a more realistic physical model, *i.e.* a kink chain that exhibits non-linear, coulombic, long-range, kink–kink interaction, in addition to a cloud of dragging point defects which shows non-stokesian viscosity behaviour. In order to determine whether the system can exhibit high-frequency harmonic generation as well as random noise production, we have performed an extensive fast Fourier transform (FFT) study of the velocity auto-correlation function [4] for several values of the normalized field variables.

2. The macro mathematical model for kink chain damping

The present macro model relies heavily on our previous treatment [5] of collective geometric kink oscillations in an atmosphere of paraelastic interstitials. According to our analytical studies, as well as modelling experiments [6], on the drag force acting on uniformly moving kinks in a cloud of Snoek- and/or Cottrell-type heavy interstitials in b.c.c. metals, we can use a Debye-type function for the power dissipation term in the equation of kink motion. The equation of motion of an individual kink in the geometric kink chain can be written as

$$M_k\partial_{tt}^2 y^i + B_k \frac{A_i\partial_t y^i}{1+A_i^2(\partial_t y^i)^2} = ba_k\sigma_r \sin(\omega t) + \sum_{i=j} F(y^i - y^j),\ i=2, 3, 4, \ldots N_k - 1 \qquad (1)$$

where the interaction force $F(y^i - y^j)$ should be modified at the leading kinks ($i=1$ and N_k) to take into account the pinning strength with respect to the nodal points. In this equation, M_k is the effective mass of a kink, y^i is the coordinate of the ith kink on a dislocation, B_k is the viscosity for the kink motion in the newtonian region, A_i is the inverse Snoek jump velocity given by $A_i = \tau_s/a_0$, τ_s is the Snoek relaxation time, σ_r is the resolved shear stress in the slip plane of the dislocation,

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b is the magnitude of the Burgers vector, a_0 is the lattice spacing, a_k is the spacing between neighbouring Peierls valleys and ω is the oscillation frequency of the external drive.

By using the following transformation of variables, $\omega t = \tilde{t}$ (scaling) and $\omega A_t u^i = y^i$ (stretching), where we have scaled the time with respect to the driving frequency and also stretched the displacement (space) with respect to the length travelled by an interstitial species during one period of motion, the following dimensionless set of differential equations can be obtained (where $i = 2, 3, \ldots, N_k - 1$)

$$y_i'' = (\tilde{\tau}_s \tilde{\Omega}_A{}^2 F_s) \sin(\tilde{t}) - (\kappa \tilde{\tau}_s \tilde{\Omega}_a{}^2) \frac{y_i'}{1 + y_i'^2} + \tilde{\tau}_s \tilde{\Omega}_a{}^2 F_{\mathrm{Bias}} + \left(\frac{L^2}{\pi^2}\right) \tilde{\Omega}_A{}^2 \frac{y_{i+1} - 2y_i + y_{i-1}}{d^2} \,\mathrm{NLF} \qquad (2)$$

where NLF is the non-linearity factor (anharmonicity) given explicitly in ref. 5. In eqn. (2), $L = L/a_0$ is the scaled dislocation segment length and $d = d/a_0$ is the equilibrium (normalized) kink–kink distance. $\tilde{\Omega}_A$ represents the free oscillation frequency of an undamped system in the linear regime (NLF $= 1$) which is normalized with respect to the frequency of the harmonic drive, *i.e.* $\tilde{\Omega}_A = \omega^0/\omega$, where we have the following classical expression, $\omega^0 = (K_\kappa/M_k)^{1/2}$. K_k is the stiffness constant of the coulombic chain in the linear region, F_s is the driving force amplitude given by $F_s = F_\kappa/F_{su}$ and F_{su} is the static force necessary for the displacement of a kink for one lattice spacing (given by $F_{su} = a_0 K_\kappa$). We also have $\kappa = B_\kappa/F_{su}$, and $\tilde{\tau}_s = \tau_s \omega$, the normalized Snoek relaxation time. κ is a very important system parameter, and represents the coupling ratio between the interstitial–kink interaction and the kink–kink mutual coupling.

3. The power spectral density associated with the kink chain

In ref. 5, the concept of the internal friction coefficient, or better the Q^{-1} factor, of the dissipative oscillator is developed. Here, we are strictly concerned with the power spectral density $S(\omega)$ associated with a kink chain under non-linear forced vibrations. This can be found as follows: (1) generate the discrete time series of velocity $\{Y_r'\}$, $r = 0$–N, by sampling the records at time interval $\Delta = T/N$; (2) calculate the mean value, and then generate the new sequence with zero mean; (3) calculate the discrete Fourier transform (DFT) of the series, $\{Y_k'\}$; (4) calculate the required series of spectral coefficients by performing the appropriate product: $S_k = |Y_k'|^2$; (5) calculate estimates of the continuum spectrum from the formula $S(\omega_k) = T/2\pi S_k$, where $\omega_k = 2\pi k/T$ rad s^{-1} and π/Δ is the Nyquist frequency that gives the upper limit for the reliable frequency range; (6) carry out final smoothing by calculating the average of adjacent spectral estimates, where T is the record length and N is the number of data points. In our computer simulations, we have the selection, $\Delta = 0.01$, $N = 2^{13}$ and a smoothing index $n = 0, 1, 2$, that yields the required bandwidth according to the formula, $B_e = (2n + 1)/T$. The time series are initially shaped by a cosine taper data window.

4. Results and discussion

During simulation work, we synthesized a new version of the Adams–Moulton procedure, which starts with the Runge–Kutta fifth-order, six-stage accurate method. The set of ordinary differential equations represented by eqn. (2) is a stiff set of differential equations, especially when we are dealing with the relaxation mode, where the shortest time constant is normally given by $t_1 = 2/t_B \tilde{\Omega}_A{}^2$, which becomes as small as 2×10^{-4} and 2×10^{-6} when $\tilde{\Omega}_A = 10$ and $\tilde{\Omega}_A = 100$ respectively.

In Fig. 1, the internal friction coefficient is plotted *vs.* the normalized Snoek relaxation time $\tilde{\tau}_s = \tau_s \omega$ or the inverse temperature on a semi-logarithmic scale for various values of the stress amplitude parameter F_s in the region of heavy damping which is called the relaxation mode. As can be seen from this figure, the kink chain model of dislocation damping shows an anomalous stress amplitude dependence, *i.e.* an increase in the stress amplitude results in a decrease in the

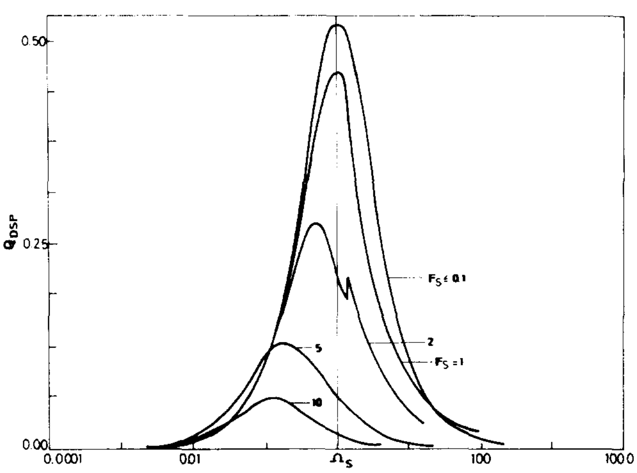

Fig. 1. Internal friction coefficient plotted as a function of the normalized Snoek relaxation time for various values of the stress amplitude F_s for the relaxation mode. This figure shows an anomalous stress amplitude dependence, and also saturation behaviour of the internal friction for high interstitial concentration. The sudden jump on the damping curve for $F_s = 2$ is due to the atmospheric tearing phenomenon. Parameters: $F_{\mathrm{Bias}} = 0$, $L = 100$ and $N_k = 3$ (the normalized resonance frequency $\tilde{\Omega}_A = 10$).

internal friction coefficient above a certain threshold level. Below this threshold stress level, which is directly proportional to the concentration of interstitials in the bulk, the dislocation damping reaches a saturation stage. The sudden jump in the damping curve, labelled as $F_s = 2$, is closely associated with the phenomenon of atmospheric tearing [3].

The power spectral density, which is taken at the peak temperature of the dislocation damping curve associated with the saturation stage, namely $\tilde{\Omega}_B = 1$, for several values of the stress amplitude, is depicted in Fig. 2. This figure shows very clearly that a strong odd-harmonic generation occurs as a sharp peak in the vicinity of the natural resonance frequency of the kink chain, $\tilde{\Omega}_A = 20$, together with some broad-band noise, at moderately high values of the strain amplitude. For higher values of the stress amplitude, such as $F_s = 25$ and 50, the system shows even-harmonic generation in the vicinity of the driving frequency with a complete loss of high-frequency odd harmonics in the presence of large-amplitude broad-band noise.

In Fig. 3, the power spectral density of a kink chain with a high natural resonance frequency is given for various values of the stress amplitude in order to illustrate the dynamic behaviour. This figure clearly shows that, if the driver frequency is very much lower than the natural frequency of the system, no odd-harmonic generation occurs at high frequency, and only the formation of broad-band noise, together with the first even-harmonic, is observed.

In order to study the character and fine features of the broad-band noise developed at low driving frequency, such as $\tilde{\Omega}_A = 50$, Fig. 4 is presented which

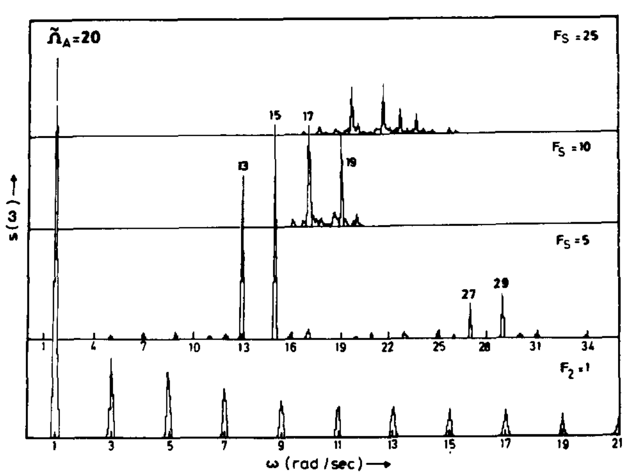

Fig. 2. Power spectral density plotted as a function of the normalized frequency (in terms of external drive) for various values of the stress amplitude F_s. This figure indicates the generation of odd harmonics in the vicinity of the natural resonance frequency ($\tilde{\Omega}_A = 20$) of the kink chain at moderate values of the stress amplitude, and the formation of broad-band noise with sharp peaks at very high values of F_s. Parameters: $F_{\mathrm{Bias}} = 0$, $L = 100$, $N_k = 3$ (data recorded at $\tilde{\Omega}_B = 1$).

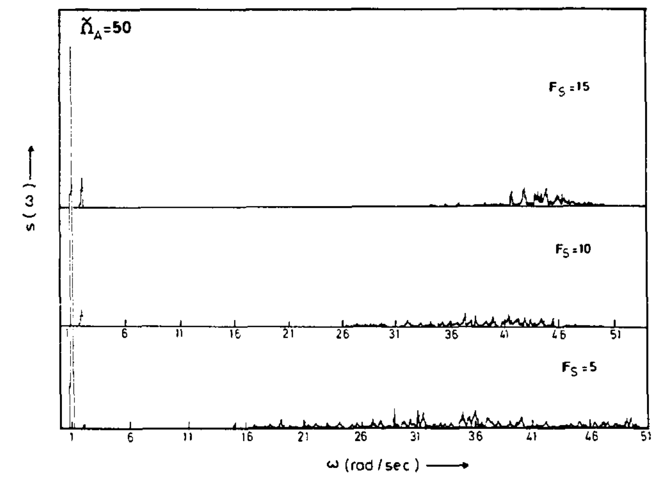

Fig. 3. Power spectral density plotted as a function of the normalized frequency for various values of the stress amplitude F_s, where the system is driven in the high natural resonance frequency mode, $\tilde{\Omega}_A = 50$. This figure indicates the complete depression of odd harmonics, and the generation of broad-band noise shifting towards the resonance frequency region. Parameters: $F_{\mathrm{Bias}} = 0$, $L = 100$, $N_k = 3$ (data recorded at $\tilde{\Omega}_B = 1$).

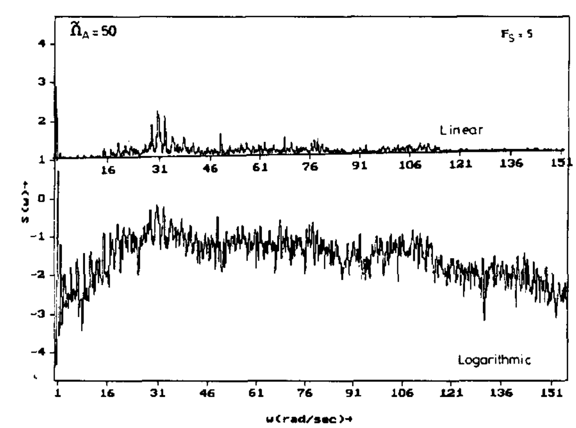

Fig. 4. Power spectral density plotted on a semi-logarithmic scale as a function of the normalized frequency for the moderate stress amplitude $F_s = 5$ and relatively low driving frequency $\tilde{\Omega}_A = 50$. This figure shows broad-band noise at high frequencies with relatively weak, but sharp, spectral lines. Parameters: $F_{\mathrm{Bias}} = 0$, $L = 100$, $N_k = 3$ (data recorded at $\tilde{\Omega}_B = 1$; smoothing index, 2).

shows the chaotic behaviour of the system at relatively moderate values of the stress amplitude, $F_s = 5$. The sharp peaks, which are more clearly detected in the linear plot, are due to periodic states which may be related to a general class of recursion relations studied by Feigenbaum [7].

5. Conclusions

We have shown that high-frequency harmonic generation and chaotic behaviour are expected to occur in strongly non-linear dissipative systems in the presence of periodic fields. The phenomena described may be found in solids whose anharmonic (or non-linear dissipative) degree of freedom can couple to a periodic field. Two probable candidates are weakly pinned charge density waves (CDW) in anisotropic solids [8] and superionic conductors [9].

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