How much illustrative can we expect an ideal system to be, which is regarded as the simplified model of a real physical phenomenon? The answer to this question is relevant in view of the successful applications of such models throughout the history of physics. The Kronig Penney model of band structure, Ising model for magnetic systems, liquid drop model of atomic nucleus, cellular automata model of self-organized criticality etc. are some of the revolutionary models with remarkable achievements. The Frenkel Kontorova (FK) chain [1,2] is one such celebrated model dealing with the mechanics of discrete nonlinear systems. Conventionally, this model has successfully been employed in studying a wide range of physical phenomena like the physics of dislocations [3] and cations [4] in metals, adsorption of atoms on crystal surface [5], magnetic structures [6] etc. In addition, it has also rendered rich understanding of processes like colloidal friction [7] and biopolymers [8,9] in recent years.

The FK model consists of a linear chain of particles connected by springs and placed over a substrate potential. In its most elementary form, the springs are assumed to be Hookean, while a sinusoidal substrate potential is considered. It was first envisaged [1,2] to represent the dislocation core as a kink in the FK chain. In particular, the existence of a threshold force to move the kink directly corresponds to the Peierls stress [10] for the dislocation motion. The Peierls stress for a dislocation is often computed by means of atomistic simulation [11-13], where the incremental shear stress (or strain) is applied quasi-statically to the crystal at \( T = 0 \text{ K} \) until the dislocation moves to the next lattice site from the previous one. Similar quasi-static simulation of the FK chain [2,14] also yields the minimum force required to move the chain. Thus, the FK model thematically depicts the mechanism of crossing the Peierls barrier in perspective of discreteness and nonlinearity intrinsic to the lattice. Nevertheless, it is obscure whether this simplified model is capable of providing finer details of the process. A closer look into this issue is worthwhile as it would not only highlight the extent of resemblance between the realistic physical system and the representative model, but also enable us to extend the applicability of the model beyond a coarse representation. In this Letter, we study the atomistic simulation of forcing a dislocation core out of its Peierls valley to obtain the atomic trajectories at sub-Burgers vector resolution. Interestingly, the simulations reveal the occurrence of intermittent relaxation bursts at such fine scale. Aiming to unfold the underlying mechanism, we apply the appropriate boundary conditions to a simple one-dimensional FK chain to let it mimic the boundary conditions used in the atomistic simulation. Even though the FK model is regarded merely as a conceptual tool subsuming the inherent discreteness and nonlinearity of the lattice, it also exhibits the abrupt bursts of structural relaxation, similar to the dislocation core. In what follows, we shall argue that such a striking feature can be perceived as the quasistatic counterpart of the stick-slip motion frequently observed in numerous dynamic systems [15,18]. In addition, the technique of principal component analysis (PCA) [19] has been used in an innovative way to establish the correspondence between a real physical system and its ideal model of lower dimensionality.

The Peierls stresses, which are defined at absolute zero temperature, have been computed here [20] for the four metals, molybdenum, iron, aluminium and copper. The simulation scheme is akin to that used in the earlier measurements [11,13]. An edge dislocation is introduced in a slab of finite thickness with periodic boundaries along the directions of dislocation line and Burgers vector. The \( x, y \) and \( z \) dimensions of the b.c.c. simulation cells are \( 90.5a(111)/2 \), \( 40a(101) \) and \( 5a(121) \), where \( a \) is the lattice constant. The Burgers vectors and the dislocation lines are along the \( x \) and \( z \) directions respectively [see the
In this study, the b.c.c. metals Mo and Fe are simulated using the modified Finnis-Sinclair interatomic potential [22], whereas the glue potential [24] and an embedded atom model [24] are used for Al and Cu respectively. In spite of a variety of potentials used in these computations, the relaxation bursts can be observed in all the studied systems. This suggests that the origin of these bursts lies rather in a more fundamental physical phenomenon, than in the complexities of the potential models employed in the simulations. In this context, the possibility of closely investigating the FK model arises as it reflects the basic features of a dislocation core, namely, the nonlinear nature of interactions and discreteness of the lattice. The potential energy of a finite FK chain with \(N\) connected particles is

\[
U = \sum_{i=1}^{N} \left[ \frac{1}{2} (x_{i+1} - x_i - l)^2 + E (1 - \cos \frac{2\pi i}{b}) \right],
\]

where the first term denotes the harmonic spring potential with \(x_i\), the position of the \(i^{th}\) particle, \(l\), the equilibrium length of each spring and \(\kappa\), the spring constant. The second term represents the periodic substrate potential where \(b\) and \(E\) are the periodicity and magnitude of the potential respectively. Here we assume the natural length of the springs connecting the adjacent atoms to be equal to the periodicity of the substrate potential (i.e., \(l = b = 1\) arb. unit). At this point, it should be noted that despite its success in demonstrating the origin of the Peierls barrier, the FK chain does not exhibit a direct correspondence to the dislocation core in all aspects. For instance, the long range interactions between two dislocations is in clear contrast to the exponential short range kink-kink interactions in the FK chain [2]. Thus, a judicious choice of boundary conditions and parameters of the FK chain is necessary so that the system can distinctly show the features of interest. In the atomistic simulations, the top and bottom surfaces of the crystalline slabs were kept fixed during the relaxation process so that the system could not revert back to the previous state of shear strain. To implement this on our FK chain, we fix both the extent of aggregate core displacement at the \(n^{th}\) step of incremental shear strain with respect to the previous step as

\[
\Delta = \sqrt{\sum_{i=1}^{N_c} |r_i(n) - r_i(n-1)|^2}.
\]

These differential displacements of the dislocation cores are plotted with the shear strains in Figs. 1(b-e). Surprisingly, one can identify the intermittent relaxation bursts characterized by narrow peaks in the profiles. Obviously, a small value of \(\Delta\) means that \(r_i(n) \approx r_i(n-1)\) implying only a small structural change in the dislocation core from the previous step of applied strain, whereas a larger value is indicative of drastic structural rearrangement. This proves that instead of exhibiting a continuous response to the incremental strain, the dislocation core structure remains almost locked in between two successive bursts. This quasistatic phenomenon is apparently analogous to the stick and slip states of dynamic variables in many physical processes of interest.

As the process of applying incremental shear strain is followed by relaxation, the atomic structure tends to reconfigure so that the potential energy of the system is minimized. The core structure can be specified by a set of \(n_e\) vectors, say \(\{r_i\}\) \((i = 1, 2, .., n_e)\), where \(N_c\) is the number of atoms in the dislocation core. We can now quantify
of its ends, thereby yielding a fixed length and fixed density condition. We accommodate $N$ particles in $N_v$ valleys so that the coverage parameter $N/N_v$ is close to $\frac{1}{2}$ to approximately resemble the local coverage due to the extra half-plane of atoms at the core of an edge dislocation. The chain is gradually shifted in small steps of $\delta$ and relaxed after each shift keeping the first and the last particles rigid during the relaxation process. Hence, the net shift of the chain at the $n^{th}$ step can be represented by the coordinates of the fixed end particle as $\Phi = x_1 - n\delta$, where the incremental shift ($\delta$) should have been infinitesimally small for the ideal quasistatic process. However, due to the trade-off between computational time and resolution, a small value of $\delta = 10^{-2}$ (arb. units) is chosen and found to be sufficient to produce the requisite spatial resolution. Moreover, in the present case of smooth periodic substrate potential, the simple steepest-descent algorithm reasonably yields the relaxed states.

The differential displacements are now computed for the particles of the FK chain for different $E/\kappa$ ranging from 0.01 to 0.1. Fig. 2(a) shows the differential displacement for $E/\kappa = 0.01$ as a function of the shift, $\Phi$, imparted to the chain where a continuous wavy nature can be observed. In addition, the change in the lengths of the connecting springs in between two successive steps is shown in Fig. 2(b), where the change is noticed along the entire chain. With increase in the value of $E/\kappa$, this wavy nature changes to relaxation bursts characterized by the intermittent peaks, which can be seen from Fig. 2(c) for $E/\kappa = 0.035$. Remarkably, these peaks which demonstrate the phenomenon of quasistatic stick-slip are present here also, similar to those in Figs. 1(b-e). Corresponding changes in the lengths of springs, which are confined to the regions near the fixed ends of the chain [Fig. 2(f)] are also intermittent and synchronized with the occurrence of relaxation bursts.

For the FK chain in its ground state, the minimum distance of the particle from the nearest maximum of the substrate potential has been used as an order parameter by Coppersmith and Fisher to characterize the Aubry-transition and breaking of analyticity [2]. For the plot shown in Fig. 2(c), $E/\kappa$ is large enough to cause the breaking of analyticity. However, in this study we encounter another variable $\Phi$, denoting the extent of shift in the chain, which determines the ground state configuration of the entire chain. Therefore, the order parameter given by $\Psi = \min|\delta_i (mod\ 1) - 0.5|_{i\neq 1,N}$ has been computed and displayed in Fig. 2(h) as a function of $\Phi$. A finite non-zero value of $\Psi$ signifies the span of re-
region around the top of the substrate potential where the presence of a particle is forbidden. It is noticeable that despite the apparently sudden occurrences of relaxation bursts, the instant of peak in Fig. 2(c) is always preceded by a gradual drop in $\Psi$ [Fig. 2(h)] during the stick state, thereby indicating the gradual narrowing of the forbidden region. Thereafter a discontinuous jump in $\Psi$ coincides with the transition to slip state at which the relaxation burst occurs. This is indicative of abrupt broadening of the forbidden regions and consequently, we expect at least one particle to suddenly cross over the peak of the substrate potential (see the schematic in Fig. 3) thereby causing a steep rise in the differential displacement profile. In addition, Fig. 2(h) also shows three instances where $\Psi$ drops and reaches values close to zero, and then rises continuously. Because of this continuous change in the order parameter, we observe small humps in the differential displacement profile which is in sharp contrast to the abrupt peaks, where the rise in $\Psi$ is discontinuous. This can be somewhat difficult to identify, for example, during the second hump (H2), where it coincides with occurrence of fifth peak (P5) in the observed profile.

Typical ground state configurations of the FK chain is given in Fig. 4(a), where most of the particles follow a structural pattern associated with a highly stable energy state and attempt to maintain it despite the incremental change in $\Phi$. As a result, the local configurations near the two fixed ends is out of skew with the rest of the chain and total energy of the system increases until the next relaxation burst. During this stick state the differential displacement of particles are found to be negligibly small and hence, the coordinates of the particles, $x_i (\text{mod } 1)$ after relaxation, when plotted with respect to the coordinates before energy minimization show the linear behavior [Fig. 4(b)]. However, during a relaxation burst some of the coordinates are knocked out of the straight line pattern, as shown in Fig. 4(c). As predicted earlier, there is always one or more particles which cross the peak of the substrate potential corresponding to $x_i (\text{mod } 1) = 0.5$ as marked in the figure.

The FK chain presented here is a 1-D model of an essentially 3-D atomic structure of a dislocation in crystal. Each and every relaxation burst always drives the chain in a forward direction as both ends are shifted in same direction. Similarly, it must be ascertained that the relaxation bursts as observed in the atomistic simulation of dislocation core also drive the core in an effectively forward direction. The notion of directionality is trivial in the FK model because of the inherent single dimensionality associated with the structure. However, the motion of a dislocation can be perceived only on a coarse scale of length, where the dislocation hops from one lattice site to another. On a sub-Burgers vector scale of length, it is difficult to associate a sense of unidirectional motion to the self-assembly of core atoms within the same Peierls valley unless a specific directionality is ascribed to it. Clearly, the conventional technique of describing the core position as the center of mass of all the core atoms (Refs. 27, 28 for example) lacks the requisite resolution and alternative data mining tool needs to be explored. In this scenario, we opt to use the PCA as a prolific tool capable of providing a high degree of compressibility of a high dimensional data and furnish its projection on a hyperspace of reduced effective dimensionality. The versatility of the PCA is reflected in its successful applications across a wide range of studies etc. In the present case of atomistic simulations, the coordinates of core atoms are recorded at each step of incremental shear strain and this strain series data is arranged as a $n_s \times 3n_c$ matrix, where $n_s$ denotes the number of strain steps and $n_c$ is the number of core atoms. Now each of the $3n_c$ columns is separately mean centered and the mean-deviation matrix thus formed is used to generate the covariance matrix [19]. Diagonalization of the covariance matrix yields the eigenvalues, and the corresponding eigenvectors. Interestingly, for all the metals under study, the largest normalized eigenvalues are always found to be in excess of 90%. Such large values conclusively prove a high compressibility intrinsic to these sets of multi-dimensional data. The projections of the datasets along the principal directions corresponding to the largest eigenvalues are presented in Fig. 5 for Mo and Al, for example. The sudden jumps present in these devil’s staircase-like profiles are synchronized with the occurrence of peaks in Fig. 1(b) and (d) and are typical signatures of the stick-slip process (see the first and

![FIG. 4: (color online). (a) Two typical ground state configurations of the FK chain ($\Phi=0, 0.9$) with $N = 91$ particles in $N_c= 60$ valleys for $E/\kappa = 0.035$. The relaxed coordinates of the particles (b) just before and (c) at the instant of occurrence of the peak P5 in Fig. 2(c) plotted with respect to the unrelaxed coordinates. The particles which have crossed the maxima of the substrate potential i.e., $x_i (\text{mod } 1) = 0.5$ (shown by dotted horizontal line), are identified in the rectangular frame.](image-url)
second panels of Fig. 4 in Ref. [9]. Moreover, one can also observe that each monotonic jump in the projected profile always causes a translation in the same direction, thereby offering a ground for comparison with the FK model.

To conclude, we have shown that at sub-Burgers vector resolution, intermittent relaxation bursts occur in the quasistatic simulation of dislocation core. Similar features are observed for the simple one-dimensional FK chain as well. This is attributed to a transition of the system from an effective stick to slip state on account of abrupt broadening of the forbidden region around the peak of the substrate potential. During the stick-slip transition, one or more atoms cross maximum of the substrate potential and hops over the forbidden zone to cause a prominent rise in the differential displacement. Moreover, the tool of principle component analysis has been used in an innovative way to extract the effective dimensionality of the atomistic data of the dislocation core atoms. The projections of the atomic trajectories on the principle directions further corroborate the efficacy of the 1-D FK chain in revealing the complex 3-D structure of the dislocation core.

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