# STICK SLIP RESPONSE OF DISLOCATION CORE

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## Abstract

By means of atomistic simulations, we demonstrate that a dislocation core exhibits intermittent quasistatic restructuring during incremental shear within the same Peierls valley. This can be regarded as a stick-slip transition, which is also reproduced for a one-dimensional Frenkel-Kontorova (FK) chain. However, on a sub-Burgers vector scale of length, it is very difficult to assign a sense of unidirectional motion of dislocation within the same Peierls valley and the conventional techniques of describing the dislocation core position lacks the essential resolution. In this scenario, we have applied the technique of principal component (PCA) analysis in an innovative way to establish the correspondence between a real physical system and its ideal one-dimensional model. Our analysis show that the projections of the atomic trajectories on the principle directions further corroborate the efficacy of the one-dimensional FK chain in revealing the complex three-dimensional structure of the dislocation core.

## Introduction

Dislocations are studied owing to their fundamental importance in deciding the mechanical properties of crystalline solids during plastic deformation. A dislocation can move under a shear load, but its motion suffers from several drag forces. The repetitive discrete atomic structure causes its energy to oscillate periodically with a period of Burgers vector as the dislocation glides through it. This creates an energy barrier, formally referred to as the Peierls barrier [1] at absolute zero temperature against the motion of the dislocation. Again, the strain field of a dislocation increases inversely with the distance from the center of the dislocation [1]. Subsequently, the core of a dislocation remains under such a large strain that the theory of linear elasticity fails in this region and nonlinear effects come into play. In his earlier work, Peierls [2] first attempted to resolve this issue of nonlinearity by combining the known solution of dislocation's elastic field and assuming the sinusoidal nonlinearity with lattice misfit to land up with an expression of the displacement field. Later on, analytical treatments are attempted [3] to perform summation of misfit energies followed by other modifications. It has been assumed that the dislocation core remained unaltered as it moved from one lattice site to the adjacent one. Though, a number of studies could provide conceptual understanding of dislocation motion, the actual mechanism of crossover of a dislocation core from a Peierls valley to the adjacent one under an applied shear load remains obscure at the sub-Burgers vector length scale.

Here we study the atomistic simulations of forcing a dislocation core out of its Peierls valley to obtain the atomic trajectories at sub-Burgers vector resolution. Simulations clearly show that a dislocation core exhibits intermittent relaxation bursts during incremental shear within the same Peierls valley. Thus, our analyses reveal that the core atoms undergo a peculiar stick-slip transition that has not been explored so far. Moreover, the technique of principal component analysis (PCA) [4] has been used in an innovative way to demonstrate that a specific

directionality can be associated with the structural rearrangement of dislocation core under the applied shear load.

**Simulation procedure**

We have performed molecular static simulations to compute the Peierls stress [2] at absolute zero temperature in four metals; molybdenum (Mo), iron (Fe), aluminium (Al) and copper (Cu) [5].

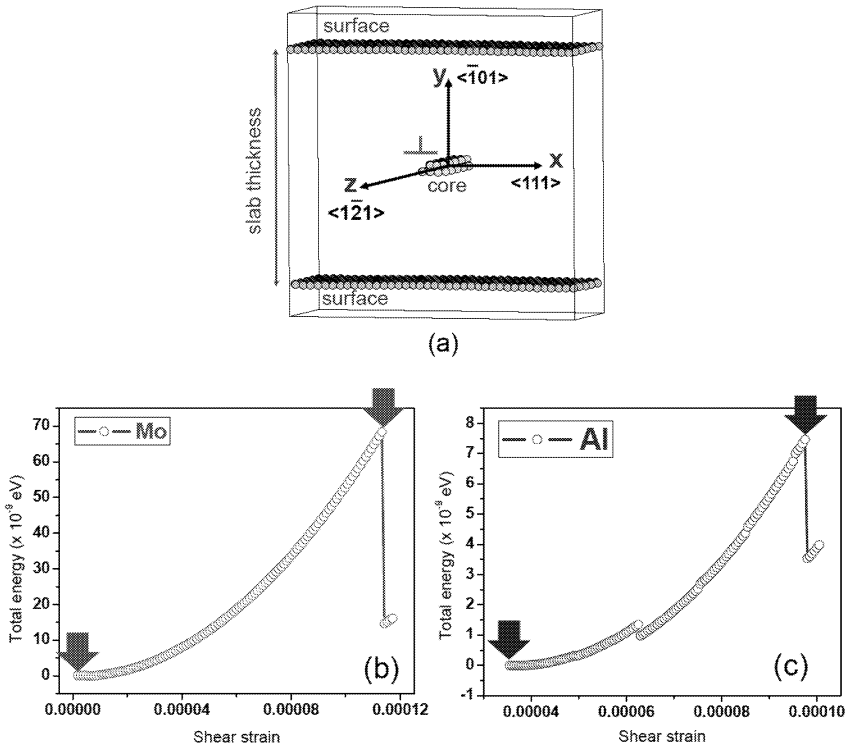


Figure 1. Typical simulation cell of (a) Mo with the edge dislocation. The crystal directions are indicated. The drastic drop in the potential energy profile is marked by the upper arrow to show the moment of crossover of the dislocation to the adjacent Peierls valley for (b) Mo and (c) Al. Simulation data between two arrows have been analyzed in each case.

The bcc metals Mo and Fe are simulated using the modified Finnis-Sinclair interatomic potential [6, 7], while the glue potential [8] and an embedded atom model [9] are employed for Al and Cu, respectively. The simulation scheme adopted here is similar to that reported in the earlier

measurements [10, 11]. An edge dislocation is introduced in a slab of finite thickness. Periodic boundary conditions are imposed along the directions of dislocation line and Burgers vector. For bcc systems the x, y and z dimensions of the simulation cell are $90.5a\langle 111\rangle/2$, $40a\langle \bar{1}01\rangle$, and $5a\langle 1\bar{2}1\rangle$, where $a$ is the lattice constant [refer Fig. 1(a)]. For fcc copper and aluminium, simulation cell dimensions are kept as $90.5a\langle 101\rangle/2 \times 20a\langle \bar{1}11\rangle/2 \times 5a\langle 12\bar{1}\rangle$. During relaxation process, we obtain a compact narrow core structure in bcc Mo and Fe, while the dislocation in Al and Cu dissociates into partials [1], as commonly observed for fcc systems. Next, the shear strain in the system is gradually increased in small steps by tilting the vertical boundary of the simulation cell. As a result, the elastic potential energy of the system increases. After each strain step, the system is relaxed to the minimum energy structure using the conjugate gradient method [10] keeping the top and bottom surfaces fixed during the relaxation. The structural potential energy is recorded for each and every individual atom at every relaxation step. As soon as the internal shear load exceeds the Peierls stress for a given system, the dislocation crosses over to the next Peierls valley giving rise to a sudden drop in the total potential energy profile [refer Figs. 1(b) and (c)]. Trajectories of all the atoms are calculated at a time step of 0.25 fs and the simulation output up to the crossover points are analyzed. To identify the dislocation core, centrosymmetric deviation parameter (CSD) [10] windows are chosen accordingly for all four metals studied here. For bcc Mo and Fe, we have used the CSD window of range 1.4–10 Å$^2$, while the ranges 3–20 Å$^2$ and 3–16 Å$^2$ are used here for Al and Cu, respectively.

## Results and discussions

During relaxation process, the atomic structure tends to attain minimum potential energy configuration. Naturally, the core atoms execute significant relaxation due to free atomic movements and larger misfits near the core whereas the linear region around the core shows negligible relaxation. To quantify the displacement of core atoms, we have measured the differential displacement as follows. If the core of the dislocation contains $n_{core}$ number of atoms, one can designate the core by specifying a set of $n_{core}$ vectors $\{r_j\}$ $(j = 1,2.....n_{core})$. Then the differential displacement at the $n^{\text{th}}$ step of strain with respect to the previous step can be expressed as $\sqrt{\sum_{j=1}^{n_{core}} \left| r_j(n) - r_j(n-1) \right|^2}$. Clearly, $r_j(n) \approx r_j(n-1)$ corresponds to small displacement and one will observe very small structural changes with respect to the previous step. After evaluating differential displacements for all the systems we found occurrence of distinct relaxation bursts. Figure 2(a) and 2(b) show, for example, the obtained profiles for Mo and Al. Instead of showing a continuous response to the incremental shear strain, the dislocation core atoms show stick-slip type of behavior between two successive relaxation bursts. It is to be mentioned that for fcc systems, the differential displacements are separately calculated for the core atoms as well as for atoms in the stacking fault regions. Interestingly, both the core atoms and stacking fault region atoms show similar relaxation bursts for Al and Cu.

Thus, our molecular static simulation results reveal that the modality of dislocation core movement resembles with stick-slip process, which is often observed in variety of physical systems and surface friction measurements [12-15]. But, all earlier studies have reported the occurrence of stick-slip dynamics at macroscopic length scales and time. This study reports a

unique stick-slip process at a much finer length scale for dislocation core, which can be regarded as the quasistatic counterpart of the stick-slip dynamics. Events like bursts and stick slip are in general associated with non-linear systems. Therefore we tried to understand these findings in light of the celebrated Frenkel-Kontorova model [16], which was first envisaged to represent dislocation core as a kink in the chain. The FK model contains linear chain of particles connected by Hookean springs in its simplest form and placed over a substrate potential. Under fixed boundary conditions we studied the relaxation behavior of this one dimensional chain in detail and could reproduce similar relaxation bursts characterized by intermittent peaks in the differential displacement profile for the FK chain. The detail results are reported elsewhere [17]. As this simple one dimensional FK chain essentially represents dislocation structure in a crystal, one important point is to be noted here. Each time the chain is pulled in a forward direction, the obtained relaxation bursts in the dislocation core also effectively moves forward and one can ascertain a sense of directionality. In atomistic simulations, the position of the dislocation core is

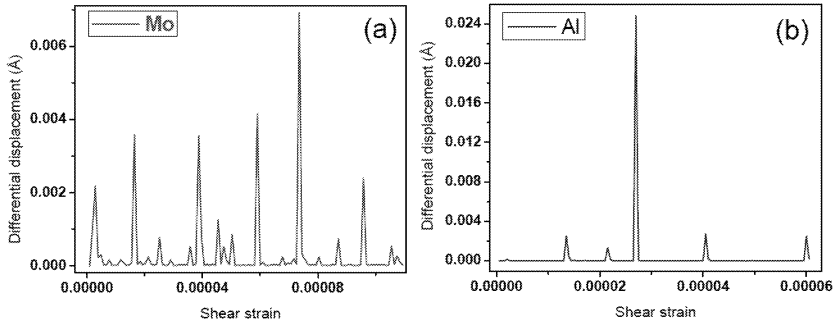


Figure 2: Distinct relaxation bursts are visible in the differential displacement of core atoms for (a) Mo and (b) Al

identified as the center of mass position of all the core atoms. The motion of a dislocation is governed by resolved shear stress, drag forces, lattice friction etc., as we have already mentioned, but the motion can only be perceived when the dislocation line glides over many lattice spacing's i.e. several Burgers vector. In that case, several drastic drops are noticed in the potential energy curve from simulation output, which conclusively prove that the dislocation has really moved to the forward direction. But, within sub-Burgers vector resolution, it is unlike to perceive a sense of 'moving dislocation' using the conventional technique of describing the core position in atomistic simulations. We now face an essential question. Is it possible to apply any dimensionality reduction analysis to the simulation data which can represent the entire core structure having single dimension? To seek answer, the technique of PCA [4] has been applied here in an innovative way. We have shown that the high-dimensional data could be compressed using PCA to give its projection on a hyper surface of reduced effective dimensionality.

The PCA technique is conventionally used to determine the variances and covariances of a multidimensional time series data which is arranged in a matrix form. In these simulations, the multidimensional data is obtained as a function of variation in shear strain, instead of a time series. The matrix is then diagonalized and one can obtain a new coordinate system where the

variances are optimized. The variances are maximum along the basis vector in this new coordinate system and it is the most significant direction representing the entire multidimensional data set as a new set of single dimension. As mentioned earlier, the coordinates of core atoms are recorded in this study at each step of incremental shear strain and this strain series data is arranged as a $n_s \times 3n_{core}$ matrix, where $n_s$ denotes the number of strain steps and $n_{core}$ is the number of atoms present in the core. The rows of these matrices consist of the x, y and z components of coordinates of $n_{core}$ atoms. The data set was considered up to the point when the dislocation remains within the same lattice site [refer Figs. 1(b) and 1(c)]. Next each of

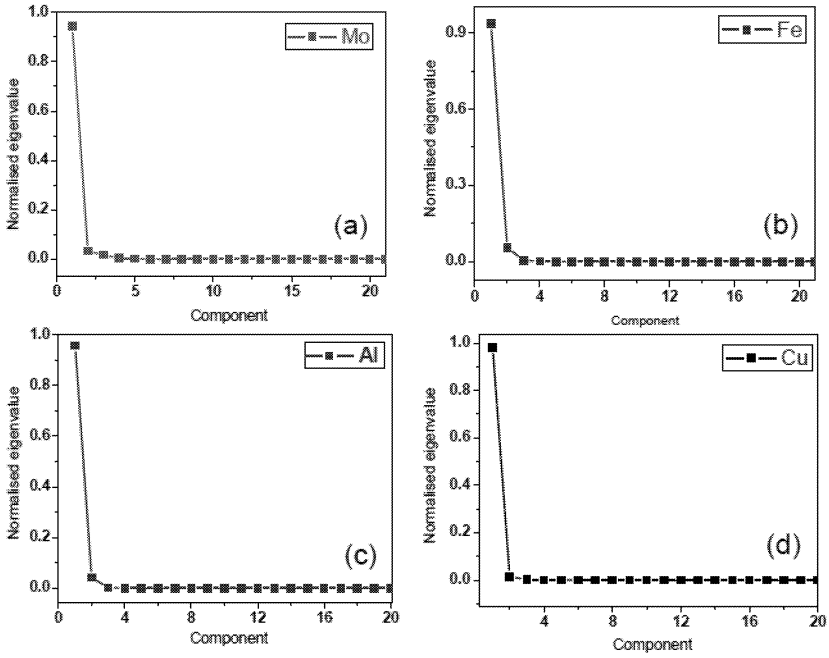


Figure 3: Normalized eigenvalues obtained from the PCA of the coordinate data of dislocation cores in (a) Mo, (b) Fe, (c) Al and (d) Cu. Only a few values are shown here as the eigenvalues drastically drop for less prominent components.

the $3n_{core}$ columns is separately mean centered and a symmetric covariance matrix is formed using this mean-deviation matrix. Diagonalization of the covariance matrix gives the eigenvalues and the corresponding eigenvectors. Total number of eigenvalues will be $3n_{core}$ in this case. The largest value corresponds to the principal direction and the variance is maximum along this direction. Our dataset yields few hundred eigenvalues for each of the four metals, but surprisingly the normalized principal eigenvalues are almost in excess of 90%. We find that remaining eigenvalues drop drastically for less significant components [refer Figs. 3(a)-(d)]. This implies a sharp directionality of dislocation core restructuring even at sub-Burgers vector

resolution along with a high compressibility intrinsic to these sets of multidimensional data. Figure 4 shows the projections of the original data on the principal directions for the largest eigenvalues for Mo, Fe, Al and Cu, where the stair-case like feature is common to all. The obtained quasiplateaus in each of these plots in Fig. 4 represent the stick states, whereas the sudden jumps correspond to the slip states. Irrespective of the magnitude of the stacking fault energy, the partial dislocations along with the stacking fault region exhibit relaxation bursts simultaneously in both Al and Cu. PCA results show that the projected profile always causes a translation of the dislocation core in the same direction, even at such a fine length scale, thereby offering a ground for comparison with the one dimensional FK model.

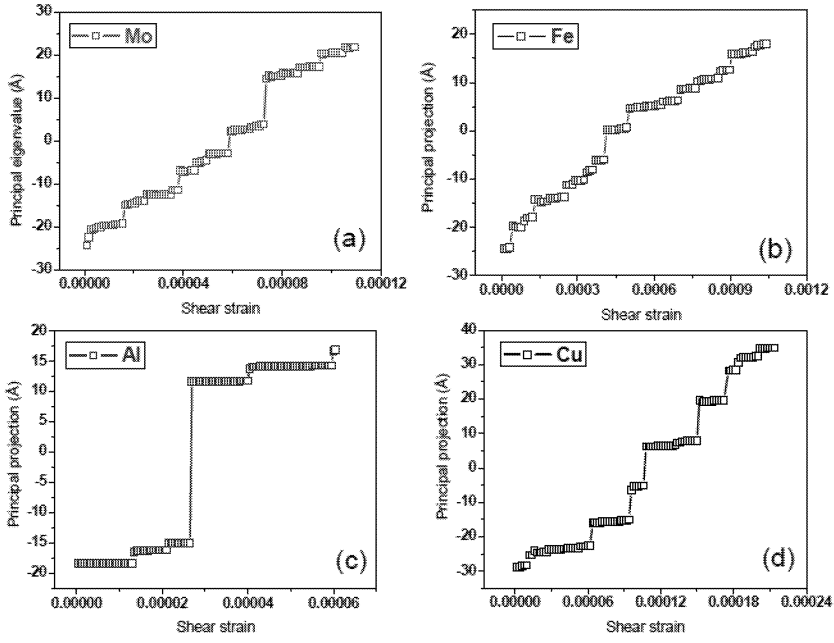


Figure 4: Obtained principal projections for (a) Mo, (b) Fe, (c) Al and (b) Cu showing staircase like profiles.

## Conclusions

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. The tool of principle component analysis has been used in a new way to extract the effective dimensionality of the atomistic data of the dislocation core atoms. One can think of associating the sense of 'unidirectional motion' of the dislocation within the same Peierls valley. Though PCA is a well known versatile technique and has been successfully used in different discipline of science, its applicability to study dislocation physics has not been explored so far. The projections of the atomic trajectories on the principle directions

further confirm that simple FK chain in one dimension is capable to reveal the complex structure of the dislocation core in 3-dimension, however, the direct link of stick-slip phenomenon in realistic systems invites further research.

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