Dynamics and nucleation of dislocations in crystals

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Periodized discrete elasticity models [1, 2, 3] are the simplest correction to linear elasticity equations allowing for nucleation and motion of dislocations in crystals. Two ingredients are needed to build a periodized discrete elasticity model for a particular type of crystal. First a linear lattice model reproducing the crystal structure and yielding the correct linear anisotropic elasticity equations in the continuum limit has to be found. To this end, an adequate potential energy for the crystal lattice is defined. This may be done by thinking of the crystal as a set of balls joined by springs or by discretizing the continuous elastic energy using the crystal lattice as a mesh. Next, the periodicity of the crystal has to be restored, allowing atoms to change neighbors. This could be done by a nonlinear relabelling protocol. From an analytical point of view, it is more convenient to introduce periodic functions of discrete differences along the primitive directions of the crystal with a period equal to the lattice constant.

These models are useful to understand nucleation and motion of dislocations (defects supported by lines) in nanocrystals at low temperatures. In heteroepitaxial growth, for instance, layers of atoms of a new crystal are grown on a substrate. After a few layers, a barrier of misfit dislocations is formed. In a different context, nanoindentation tests use the tip of an electronic microscope to apply a load on the surface of a nanocrystal. Past a critical stress, dislocations are generated around the tip. These crystals are perfect except for a few dislocations moving along primitive directions of the crystal. Secondary slip systems are only activated at large temperatures and high strain rates. Nanoindentation tests provide information on the nanocrystal mechanical properties and on incipient plasticity.

Compared to standard molecular dynamics models, the mathematical structure of periodized discrete elasticity models allows for cheaper simulations and an elementary analysis. By construction, the perfect crystal is a stable equilibrium. Pinned edge and screw dislocations are stationary solutions behaving at infinity like singular solutions of the Navier equations [1, 4]. Moving dislocations are travelling wave solutions [5]. Dislocations interact as expected. For example, if we have a set of planar edge dislocations with parallel Burgers vectors along the x axis, dislocations having the same sign of the Burgers vector repel each other. Dislocations whose Burgers vectors have opposite signs attract and they either cancel each other or form dipoles and loops. In simple geometries, a more precise analysis can be done.

Let us consider a 2D cubic lattice for which only displacements in the x direction are relevant. The lattice evolution is governed by the nondimensional equations:

$$\begin{aligned} m\frac{d^2u_{i,j}}{dt^2}+\alpha\frac{du_{i,j}}{dt} &= u_{i+1,j}-2u_{i,j}+u_{i-1,j} \\ &+ \frac{A}{2\pi}\left[\sin(2\pi(u_{i,j+1}-u_{i,j}))+\sin(2\pi(u_{i,j-1}-u_{i,j}))\right], \end{aligned} \tag{1}$$

where $u_{i,j}$ represents the dimensionless displacement of the atom (i, j) in the direction x. Periodicity is only needed in the direction in which changes of neighbours can take place. We have selected a sine function. In practice, this periodic function would have to be fitted to the material. The lattice spacing is normalized to 1. Here $A = C_{44}/C_{11}$ for a cubic crystal with elastic constants C_{11}, C_{12}, C_{44}.

This simple model allows for nucleation and motion of edge dislocations along the x direction when a shear stress of strength F is applied in the x direction. Dislocation depinning can be characterized as a global bifurcation [6], explaining the role of stationary and dynamic Peierls stresses [5, 7, 8]. Dislocation nucleation appears as a subcritical pitchfork bifurcation, yielding the critical stress for nucleation, the nucleation site and the nature of nucleated defects [9].

Dislocation depinning. Let us consider a lattice containing an edge dislocation. We apply a shear stress of strength F in the x direction. Stationary dislocation solutions are constructed by looking for stationary solutions that behave at infinity like $\theta(i, \frac{j}{\sqrt{A}}) + Fj$, θ being the angle function. For small F, the resulting solutions take values in the region where the sine function is increasing. Existence of stationary dislocations can be proven using a maximum principle for the overdamped version of (1) and constructing adequate sub and supersolutions [4]. Above a threshold, the spatial operator changes type and dislocations start to move.

Two critical values of the stress are found. Below F_s, stable stationary dislocation solutions exist. Above F_d, stable travelling dislocations are found. In general, $F_d < F_s$. Both thresholds only agree in the overdamped limit $m = 0$. In this case, a prediction of the dislocation speed is found by assembling the information available above and below threshold. The linear stability analysis of the stationary dislocation solutions shows that the largest negative eigenvalue vanishes at F_s. The corresponding bifurcation is a global saddle-node bifurcation, and the solution can be approximated by matched asymptotic expansions in the limit as $F \to F_s+$ (for $F > F_s$ the dislocation moves as a traveling wave). The amplitude equation corresponding to a saddle-node bifurcation has solutions that blow up in finite time as $F \to F_s+$. At the blow-up times, the solution described by the amplitude equation has to be matched to an inner solution that solves (1) with $F = F_s$ and appropriate matching conditions. The profiles of the travelling dislocations are step-like; see [1, 6] for details. A numerical calculation of the traveling wave shows that as F approaches F_s from above, its profile develops steps, which become steeper and steeper near F_s where the previously described approximation based on the global bifurcation applies. The speed of the wave is related to the time one atom spends in a step, which can be estimated using the normal form of the bifurcation. This yields a $(F - F_s)^{1/2}$ scaling for the speed. The scaling changes to 3/2 in the presence of spatial disorder. It would also be affected by temporal fluctuations, if present; see [5] and references therein. When $m \neq 0$, predicting a speed law requires the analysis of a bifurcation in the branch of travelling waves.

Homogeneous nucleation. Let us now analyze homogeneous nucleation of dislocations by shearing a dislocation-free state. When $F = 0$, $u_{i,j} = 0$ is a stable solution corresponding to a perfect crystal. As F is increased, we find a branch

BR0 of stationary solutions representing sheared lattices without defects. Numerical continuation indicates that this brach becomes unstable at a critical shear stress F_n. At this point, a subcritical pitchfork bifurcation takes place. Two new branches of stationary configurations, BR1 and BR2, appear. Both are initially unstable, but become stable for stresses larger than F_n^1 and F_n^2, respectively. BR1 represents nucleation of one dipole, which splits in two edge dislocations moving towards the boundary of the lattice. BR2 corresponds to nucleation of two dipoles, that split in four edge dislocations. Since F_n^1 and F_n^2 are smaller than F_n, nucleation can occur before reaching F_n. The final pattern observed in dynamical tests depends on the way the load is applied. If we deform a lattice at a large strain rate, one dipole is nucleated. At low strain rates, two dipoles are observed. The eigenfunction corresponding to the zero eigenvalue of the linear stability problem at F_n locates the nucleation site. Nucleation starts in the region where the eigenfunction takes large values. The two different patterns correspond to perturbations of the lattice configuration at F_n by either adding or subtracting multiples of the eigenfunction. Dipoles split because the critical stress for nucleation is much larger than the critical stress for edge dislocation depinning.

In an isotropic crystal, our critical stress for nucleation scales as $\frac{\mu}{4}$, comparable to Taylor's estimate for the theoretical strength of a crystal. The factor $\frac{1}{4}$ depends on our choice of periodic interaction. Though homogeneous nucleation has long be thought to be an elastic instability at finite strength, no precise analysis of this instability had been carried out up to now. Preliminary tests in more complex indentation or fracture settings suggest that a similar analysis is possible.

References

[1] L.L. Bonilla, A. Carpio, *Defects, singularities and waves*, Recent Advances in Nonlinear Partial Differential Equations and Applications, Serie 'Proceedings of Symposia in Applied Mathematics', **65**, AMS (2007), 131-150.

[2] L.L. Bonilla, A. Carpio, I. Plans *Dislocations in cubic crystals described by discrete models*, Physica A **376** (2007), 361-377.

[3] A. Carpio, L.L. Bonilla *Discrete models for dislocations and their motion in cubic crystals*, Phys. Rev. B **71** (2005), 134105, 1-10.

[4] A. Carpio *Wavefront solutions for discrete two dimensional nonlinear diffusion equations*, Appl. Math. Lett. **15** (2002), 415-421.

[5] A. Carpio, L.L. Bonilla *Edge dislocations in crystal structures considered as traveling waves of discrete models*, Phys. Rev. Lett. **90** (2003), 135502, 1-4.

[6] A. Carpio, L.L. Bonilla *Depinning transitions in spatially discrete reaction-diffusion equations*, SIAM J. Appl. Math **63** (2003), 1056-1082.

[7] A. Carpio *Nonlinear stability of oscillatory wave fronts in chains of coupled oscillators*, Phys. Rev. E **69** (2004), 046601, 1-13.

[8] A. Carpio, L.L. Bonilla *Oscillatory wave fronts in chains of coupled nonlinear oscillators*, Phys. Rev. E **67** (2003), 056621, 1-11.

[9] I. Plans, A. Carpio, L.L. Bonilla, *Homogeneous nucleation of dislocations in a periodized discrete elasticity model*, Europhysics Letters **81** (2008), 36001, 1-6.