Modeling and simulation: Examples in Materials and Biology

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2 Dislocations in crystals

Dislocations are line defects in an elastic crystal [6]. When a sufficiently large stress is applied, these dislocations glide along the crystallographic planes of the crystal and interact with other dislocations they find on their way. In addition, new dislocations are observed to be generated at certain nucleation sites. As a result they appear typically in very large numbers (10^{12} dislocations/cm^2 in heavily worked metals) and modify the mechanical properties of the material. In particular, dislocations are thought to control the plastic properties of crystalline solids (at low temperature).

It is well known that, under an applied stress, crystals deform elastically up to a critical value of this stress, known as the yield stress. For higher stresses, the deformation becomes plastic (irreversible) and ends up eventually in fracture. The yield stress is thought to be the stress at which large numbers of dislocations start moving. Once in the plastic regime, the generation, motion, and interaction of dislocations results in the formation of complicated networks of defects in the microscopic structure of the material. When these networks are so dense that dislocations cannot move freely, the crystal hardens (work hardening). This effect is very important when working with metals, since heavily worked metals are stronger than unworked metals.

Dislocations can be described in many different ways, depending on the lengthscale on which they are viewed. At the microscopic level, they appear as defects in the crystalline lattice. Then, if the separation between dislocations is not too small, there is a mesoscopic scale at which the dislocations may be modelled as line singularities of the elastic stress evolving in a continuous material. Finally, at a macroscopic scale containing large numbers of dislocations we can think in terms of a continuous dislocation density.

2.1 Continuous models for pile-ups

In metal plasticity, we can define an outer length scale as that on which dislocations can be regarded as a line singularity, i.e. the outer equations are the Navier equations of linear elasticity. The second order strain tensor is defined

$$\boldsymbol{\epsilon} = (\nabla \mathbf{u})^S$$

where $\mathbf{u}$ is the elastic displacement, and the superscript S denotes the 'symmetric part of'. The strain tensor is related to the stress tensor through Hooke's law

$$\boldsymbol{\sigma} = \lambda \mathrm{tr}(\boldsymbol{\epsilon})\mathbf{I} + 2\mu\boldsymbol{\epsilon}$$

where λ and μ are the Lame constants. Finally, the equations of elastic equilibrium are

$$\mathrm{div}(\boldsymbol{\sigma}) = 0.$$

An isolated dislocation can be modelled as a singular solution of these equations in which the displacement is not single valued [1]. This is the classical Volterra model of dislocations. In general, they may be characterized by their tangent vector and a microscopic parameter known as the Burgers vector, which measures the form of the local mismatch in the crystal lattice.

We obtain a model for the interaction of two families of edge dislocations. We take the first family to be tangent to the z-direction and Burgers vector in the x-direction, and the second family to have tangent in the y-direction and Burgers vector in the x-direction. Thus, the first family has the xz-plane as its slip plane, while the second family has the xy-plane as its slip plane, and if we assume that the dislocations remain rectilinear then both families will glide in the x-direction. We refer to them as 'dislocations type 1' and 'dislocations type 2', respectively. By symmetry considerations, the problem can be reduced to a one-dimensional problem [2], giving two populations with densities $w_1(x,t)$ and $w_2(x,t)$, respectively. We want to determine how these density profiles evolve with time.

Conservation of dislocations for both families yields [6]

$$\frac{\partial w_1}{\partial t} + \frac{\partial}{\partial x}(w_1 v_1) = 0,$$
$$\frac{\partial w_2}{\partial t} + \frac{\partial}{\partial x}(w_2 v_2) = 0,$$

where v_i is the velocity of family i. Then, in the absence of any interaction between the families we would close the model with velocity laws such as

$$v_1 = \text{sign}(\sigma_{1,2})|\sigma_{1,2}|^{\gamma},$$
$$v_2 = \text{sign}(\sigma_{1,3})|\sigma_{1,3}|^{\gamma},$$

In our setting, the first family of dislocations can be seen as a set of lines parallel to the y-axis, and the second family is another set of lines parallel to the z-axis. Both families move along the x-axis. However, as dislocations from the first family move they must cut through the dislocations of the second family. We suppose that there is a strong resistance to this cutting depending on the density and we consider [2] velocity laws of the form

$$v_1 = \text{sign}(\sigma_{1,2})(|\sigma_{1,2}| - a\sqrt{w_1}),$$
$$v_2 = \text{sign}(\sigma_{1,3})(|\sigma_{1,3}| - a\sqrt{w_2}),$$

with $a > 0$. This is a system of conservation laws that may change type form hyperbolic to elliptic. This corresponds to the onset of pattern formation, formation of dislocation pile-ups. When regularized, we obtain a free-boundary parabolic problem describing the process [6].

2.2 Lattice models for isolated defects

An elementary model for dislocation dynamics in crystal lattices is provided by Frenkel-Kontorova type equations for the displacement $u_n(t)$ of atoms from their equilibrium position along a row in a cubic lattice

$$m u_n'' + \alpha u_n' = d(u_{n+1} - 2u_n + u_{n-1}) - A g(u_n) + F.$$

All the parameters are positive: m represents the atom mass, α friction, d elastic springs between atoms (interaction strength), F applied force to set the defect in motion. $g(u_n)$ is a periodic function, whose period is given by the lattice constant a. At equilibrium, all atoms are located at lattice positions separated by a distance a in cubic lattices. Dislocations in this framework are represented by a front like solutions, that is, solutions that grow from a stable zero $z_1(F/A)$ of $-Ag(z) + F$ to the next stable zero $z_3(F/A)$, passing through the instable zero $z_2(F/A)$. When $F = 0$, $z_1(F/A) = 0$ and $z_3(F/A) = a$.

If friction is high, the motion is overdamped and we may set $m = 0$ to study it. Once can find a threshold $F_c(A)$ such that [3]

- If $|F| \leq F_c(A)$, there are stationary wave front solutions u_n increasing monotonically from $z_1(F/A)$ at $-\infty$ to $z_3(F/A)$ at ∞.
- If $|F| > F_c(A)$ and is close to A, there are traveling wave front solutions $u_n(t) = u(n - ct)$ with wave speed $c(F)$ and profile $u(z)$ solution of

  $$-cu(z) = u(z-1) - 2u(z) + u(z+1) - Ag(u(z)) + F$$

  increasing monotonically from $z_1(F/A)$ at $-\infty$ to $z_3(F/A)$ at ∞. This solution is unique modulo translations.
- traveling and stationary wavefronts cannot coexist.

Stationary wavefronts represent pinned dislocations. Traveling wavefronts represent moving dislocations. $F_c(A)$ represents the Peierls stress needed to move dislocations in the lattice. As $|F| \to F_c(A)$, $c(F) \to 0$, the profiles $u(z)$ develop steps and become discontinuous at $F_c(A)$. This fact is related to a global bifurcation in the system, which is locally of saddle node type and can be used to estimate velocities as $|c(F)| \sim \alpha(F_c)(|F| - F_c(A))^{1/2}$, see [12].

In the absence of friction, or for small friction, we must study the problem with inertia. For piecewise linear g, for instance, $g(u) = u + 1$ if $u < 0$ and $g(u) = u - 1$ if $u > 0$, it is possible to construct explicitly all the branches of traveling wave solutions [15]. In this case, the wave front profiles develop wavy tails. In principle, different wave profiles and speeds are possible. In practice, stability can be proven [16] for a family which displays oscillations only in one tail, the leading edge is monotonic and whose speed surpasses a critical value. We identify two thresholds, the static Peierls stress $F_c(A)$, and the dynamic Peierls stress $F_d(A)$. As before, stationary wavefronts exist when $|F| \leq F_c(A)$. Traveling wavefronts exist when $|F| > F_d(A)$. Both coexist for $F_d(A) < |F| < F_c(A)$. Thus, the system displays hysteresis. As we increase the applied force from zero, wavefront solutions representing dislocations start too move when the force magnitude surpasses $F_c(A)$. Once the lattices dislocation is moving, we can decrease the force below $F_c(A)$, it will still move until it falls below $F_d(A)$.

We can study two dimensional dislocations in a cubic lattice by means two dimensional lattice models [11, 14]. In the simplest version, the displacement of the lattice points $u_{i,j}(t)$ in the direction of motion (say, the direction x) is governed by

$$\frac{\partial u_{i,j}}{\partial t} = u_{i-1,j} - 2u_{i,j} + u_{i+1,j} + A(\sin(u_{i,j-1} - u_{i,j}) \sin(u_{i,j+1} - u_{i,j})), \ A > 0.$$

Solutions representing dislocations can be generated using elastic far fields of dislocations as initial and boundary conditions [11]. The system relaxes to stationary solutions that represent the corresponding lattice distortion. For instance, if we choose initial and boundary conditions given by $s_{i,j} = \theta(i, j/\sqrt{A}) + Fj$ where θ is the angle function from 0 to 2π and $F > 0$ is a control parameter, we obtain stationary solutions representing edge dislocations for small F. As F grows, stationary solutions will disappear and traveling patterns will be observed [14]. Notice that if we linearize the spatial operator about $s_{i,j}$, we have a discrete elliptic problem for F small but it changes type as F grows.

The idea can be extended to fully 2D and 3D situations by developing 'discrete periodized elasticity lattice models' [18, 23]. We discretize the derivatives appearing the elasticity stress tensor with the required crystal symmetry by means of finite differences in the principal lattice directions, with step equal to the lattice constant, and then periodize, that is, we replace them by periodic functions of the differences, with lattice period. Then, we derive the motion equations with the resulting discrete and periodic stress tensor. For instance, in two dimensions we find

$$\begin{aligned} M u_1'' &= C_{11} D_1^- [g(D_1^+ u_1) g'(D_1^+ u_1)] + C_{12} D_1^- [g(D_2^+ u_2) g'(D_1^+ u_1)] \\ &\quad + C_{44} D_2^- [(g(D_2^+ u_1) + g(D_1^+ u_2)) g'(D_2^+ u_1)], \\ M u_2'' &= C_{11} D_2^- [g(D_2^+ u_2) g'(D_2^+ u_2)] + C_{12} D_2^- [g(D_1^+ u_1) g'(D_2^+ u_2)] \\ &\quad + C_{44} D_1^- [(g(D_1^+ u_2) + g(D_2^+ u_1)) g'(D_1^+ u_2)]. \end{aligned}$$

Similar equations are derived for 3D lattices. Dislocation solutions of the corresponding lattices are generated using the known elastic far field for each type of crystal [18, 23].

2.3 Nucleation in lattices

We can use discrete periodized elasticity models to gain insight on the mathematical processes behind defect nucleation. Unlike the models used for large scale molecular dynamics simulations, which implement cut offs to reduce the computational cost, these models involve smooth nonlinearities and are amenable to analysis.

Consider a bidimensional cubic lattice of lattice constant $a = 2\pi$. Let $u_{i,j}(t)$ be the displacement of point (i, j) in the x direction, governed by

$$\begin{aligned} m \frac{\partial^2 u_{i,j}}{\partial t^2} + \alpha \frac{\partial u_{i,j}}{\partial t} &= u_{i-1,j} - 2u_{i,j} + u_{i+1,j} \\ &\quad + A(\sin(u_{i,j-1} - u_{i,j}) \sin(u_{i,j+1} - u_{i,j})) \end{aligned}$$

in a square lattice $i = 1, \dots, N_x$, $j = 1, \dots, N_y$. We enforce boundary conditions $u_{i,j} = F(j - (N_y + 1)/2)$. This is equivalent to 'shearing' the lattice [24]. As F grows, we observe that the initial zero solution for $F = 0$ changes into slowly varying stationary solutions until we reach a point F_c past which the lattice structure is distorted in two main different ways. Linearizing the problem at $F = F_c$ we find a zero eigenvalue for the resulting matrix, while all the eigenvalues are negative for $F < F_c$. The branch of stationary solutions $s_{i,j}(F)$ is stable. At $F = F_c$ two new branches appear. The system undergoes a pitchfork bifurcation [24].

Changing the geometry we can study other geometries, as for instance, crystal indentation by means of indenters. Now $v_{i,j}(t)$ denotes the vertical displacement, governed by

$$
\begin{aligned}
m\frac{\partial^2 v_{i,j}}{\partial t^2} + \alpha\frac{\partial v_{i,j}}{\partial t} &= v_{i-1,j} - 2v_{i,j} + v_{i+1,j} \\
&+A(\sin(v_{i,j-1} - v_{i,j})\sin(v_{i,j+1} - v_{i,j}))
\end{aligned}
$$

in a square lattice $i = 1, \dots, N_x$, $j = 1, \dots, N_y$. We set the boundary conditions representing a 'push down' from the central top part:

- Left-hand side: $v_{1,j} = v_{0,j}$.
- Right-hand side: $v_{N_x,j} = v_{N_x+1,j}$.
- Left-hand-side of the top layer ($1 \le i < p_1$): $v_{i,N_y} = v_{i,N_y+1}$.
- Right-hand-side of the top layer ($p_2 < i \le N_x$): $v_{i,N_y} = v_{i,N_y+1}$.
- Bottom layer of the domain: $v_{i,0} = 0$.
- Central atoms ($p_1 \le i \le p_2$) are pushed downwards according to: $v_{i,N_y+1} - v_{i,N_y} = -f(i)$, where f has a triangular profile, pointing downwards, with magnitude $F > 0$.

As F grows, we observe that the initial zero solution for $F = 0$ develops localized lattice distortions that travel downwards. As we decrease F to zero the distortions travel upwards and may disappear [32]. The branch of stationary solutions that starts at F develops bifurcations at specific values of F at which lattice with different distortions are created. Such new branches are stable for some ranges of F, while the defects simply travel. The configuration bifurcates at new F values, new distortions are created, that travel for while, and the process is repeated as F grows. When we decrease F, the process is reversed. Created distortions travel upwards, and disappear.

3 Propagation of biological impulses

Understanding wave propagation in discrete excitable media is challenging because of poorly understood phenomena associated with spatial discreteness. The study of the transmission of nerve impulses along myelinated axons and muscle contraction are paradigmatic examples.

3.1 Myelinated nerves

Myelinated nerve fibers, such as the motor axons of vertebrates, are covered almost everywhere by a thick insulating coat of myelin. Only a fraction of the active membrane is exposed, at small active nodes called Ranvier nodes. The myelinated axons of motor nerves can be very long, and contain hundreds or thousands of nodes. The wave activity jumps from one node to the next one giving rise to "saltatory" propagation of impulses. Saltatory conduction on myelinated nerve models has two important features. One is the possibility of increasing the speed of the nerve impulse while decreasing the diameter of the nerve fiber. The other is propagation failure when the myelin coat is damaged, which causes diseases such as multiple sclerosis.

3.1.1 Hodgkin-Huxley equations for myelinated axons

A myelinated nerve is a sequence of exposed Ranvier nodes separated by regions covered with myelin sheaths. Myelin is considered to be a perfect insulator. Then, the nerve axon can be represented by an equivalent circuit where C and R represent lumped resistance and capacitance. V_k, I_k and $I_{ion}(k)$ represent the membrane potential, internodal current and ionic current at the k-th node. Applying Kirchoff's laws to the circuit yields:

$$V_{k-1} - V_k = RI_k, \quad I_k - I_{k+1} = C\frac{dV_k}{dt} + I_{ion}(k)$$

Adopting at each node the Hodgkin-Huxley expression for the ion current, we obtain the discrete Hodgkin-Huxley model for a myelinated axon:

$$\begin{aligned} & C\tfrac{dV_k}{dT} + I_{ion}(V_k, M_k, N_k, H_k) = \\ & \overline{D}(V_{k+1} - 2V_k + V_{k-1}), \\ \tfrac{dM_k}{dT} &= \overline{\lambda}_M \overline{\Lambda}_M(V_k)(M_\infty(V_k) - M_k), \\ \tfrac{dN_k}{dT} &= \overline{\lambda}_N \overline{\Lambda}_N(V_k)(N_\infty(V_k) - N_k), \\ \tfrac{dH_k}{dT} &= \overline{\lambda}_H \overline{\Lambda}_H(V_k)(H_\infty(V_k) - H_k), \end{aligned}$$

where the index k designs the k-th node of the fiber. Here, V_k is the deviation from rest of the membrane potential, N_k is the potassium activation, M_k is the sodium activation and H_k the sodium inactivation. The ion current is given by:

$$\begin{aligned} & I_{ion}(V, M, N, H) = \overline{g}_{Na} M^3 H (V - \overline{V}_{Na,R}) \\ & + \overline{g}_L (V - \overline{V}_{L,R}) + \overline{g}_K N^4 (V - \overline{V}_{K,R}). \end{aligned}$$

The fraction of open K^+ channels is computed as N_k^4. The fraction of open Na^+ channels is approximated by $M_k^3 H_k$. The parameters have the following interpretation. $\overline{g}_{Na}$ and $\overline{g}_K$ are the maximum conductance values for Na^+ and K^+ pathways, respectively. $\overline{g}_L$ is a constant leakage conductance. The corresponding equilibrium potentials are $\overline{V}_{Na}$, $\overline{V}_K$ and $\overline{V}_L$, respectively. Then, $\overline{V}_{Na,R} = \overline{V}_{Na} - \overline{V}_R$, $\overline{V}_{K,R} = \overline{V}_K - \overline{V}_R$ and $\overline{V}_{L,R} = \overline{V}_L - \overline{V}_R$, where $\overline{V}_R$ is the resting potential. C is the membrane capacitance. The coefficient $\overline{D} =$

$\frac{1}{L(r_i+r_e)} = \frac{1}{R}$, where L is the length of the myelin sheath between nodes and r_i, r_e the resistances per unit length of intracellular and extra-cellular media.

This model is adequate for the long axons of peripheral myelinated nerves. Numerical simulations representing the propagation of nerve impulses are presented in [19], where an asymptotic construction of pulse like solutions is also given. Nerve impulse propagation is shown to fail when the leading front of the pulse is pinned [12], which happens when the myelin sheath deteriorates (multiple sclerosis) or in the presence of drugs, see simulations in [19].

3.1.2 Discrete FitzHugh-Nagumo equations

The discrete Fitz Hugh-Nagumo system is a simplification of the Hodgkin-Huxley model for myelinated nerves useful to gain qualitative understanding of the mathematical clues of successful pulse propagation and propagation failure [12, 13]:

$$\begin{aligned} \frac{du_k}{dt} &= d\,(u_{k+1} - 2u_k + u_{k-1}) + f(u_k) - v_k, \\ \frac{dv_k}{dt} &= \epsilon\,(u_k - Bv_k), \end{aligned}$$

$k = 0, \pm 1, \ldots$. Here u_k and v_K are the membrane potential and the recovery variable (which acts as an outward ion current) at the kth excitable membrane site (node of Ranvier). The cubic source term $f(u_k)$ is an ionic current, and the discrete diffusive term is proportional to the difference in internodal currents through a given site. The constant B is selected so that the source terms in the FHN system are $O(1)$ for u_k and v_k of order 1, that the only stationary uniform solution is $u_k = 0 = v_k$, and that the FHN system has excitable dynamics. The constant $\epsilon > 0$ is the ratio between the characteristic time scales of both variables. We assume $\epsilon \ll 1$, that is, fast excitation and slow recovery.

3.2 Morris-Lecar model for muscle fiber contraction

Similar models are used to describe the contraction and recovery of muscle fibers. The Morris-Lecar model is given by

$$\begin{aligned} \frac{dv_k}{dt} &= D(v_{k+1} - 2v_k + v_{k-1}) + f(v_k, w_k) - 2I, \\ \frac{dw_k}{dt} &= \lambda \cosh(\frac{v_k - V_3}{2V_4})\big[1 + \tanh(\frac{v_k - V_3}{V_4}) - 2w_k\big], \end{aligned}$$

where the index k denotes the k-th site and:

$$f(v, w) = 2w(v - V_K) + 2g_L(v - V_L) + g_{Ca}\big[1 + \tanh(\frac{v - V_1}{V_2})\big](v - 1).$$

v_k is the ratio of membrane potential to a reference potential and w_k is the fraction of open K^+ channels. The time scale is $\frac{\overline{g}_K}{2C_m}$, $\overline{g}_K$ being the K^+ conductance and C_m the membrane capacitance.

This system is a reduced version of the full Morris-Lecar model, which involves one more fast variable m_k. It exhibits a rich dynamical behavior depending on its stationary solutions. There are two possibilities. It there is a unique stable constant solution, the system displays excitable dynamics. When it happens to be unstables, the system develops self-oscillations and displays synchronization phenomena [20].

4 Propagation of electric impulses in semiconductors

Semiconductors are materials of great interest in microelectronics, and are the basis of many devices that exploit the formation of patterns and oscillations in the electric field.

4.1 Discrete models for domain walls in superlattices

Semiconductor superlattices are formed by a sequence of layers of different semiconductor materials. The dynamics of domain walls separating regions with different electric field in semiconductor superlattices is described by systems of the form

$$\frac{dE_i}{dt} + \frac{v(E_i)}{\nu}(E_i - E_{i-1}) - \frac{D(E_i)}{\nu}(E_{i+1} - 2E_i + E_{i-1}) = J - v(E_i),$$

for the electric field E_i at well i. Here, v, D are positive functions and $\nu > 0$ is large. v is a cubic, it grows from 0 to a local maximum, decreases to a positive minimum, and increases to infinity later. For a range of J, we have three zeros $z_1(J) < z_2(J) < z_3(J)$, two of which are stable. For ν large enough, we can construct wavefront solutions [4] and the situation is similar to that described for one dimensional discrete dislocation models. We find thresholds $J_{c_1}(\nu) < J_{c_2}(\nu)$ such that [8]

- If $J_{c_1}(\nu) < J < J_{c_2}(\nu)$, there are stationary wave front solutions E_i increasing monotonically from $z_1(J)$ at $-\infty$ to $z_3(J)$ at ∞.
- If $J_{c_1}(\nu) > J$ or $J > J_{c_2}(\nu)$, there are traveling wave front solutions $E_i(t) = E(i - ct)$ with wave speed $c(J)$ and profile $E(z)$ increasing monotonically from $z_1(J)$ at $-\infty$ to $z_3(J)$ at ∞. Such waves travel with speeds of opposite sign for each range of J, some of them in the same sense as electrons, some contrary to them.
- traveling and stationary wavefronts cannot coexist.

Stationary wavefronts represent pinned domain walls. Traveling wavefronts represent moving domain walls. As $J \to J_{c_1}(\nu)$ or $J \to J_{c_2}(\nu)$, $c(J) \to 0$, the profiles $E(z)$ develop steps and become discontinuous at the critical values of J. This fact is related to a global bifurcation in the system, which is locally of saddle node type and can be used to estimate velocities as $|c(J)| \sim |\alpha(J_c)|(|J - J_c|)^{1/2}$.

We can add noise $\gamma\xi_i$ to the applied current J, where $\gamma > 0$ characterizes the disorder strength and ξ_i is a zero mean random variable taking values on an interval $(-1, 1)$ with equal probability [10]. Setting $\gamma = 0$, we can repeat with this equation the study done in the previous exercise and obtain a velocity that scales like $|J - J_c|^{1/2}$. However, when we add noise, for each realization of the noise, the thresholds J_c is shifted slightly up or down by the noise. The observed velocity will be the average of the velocities observed for a large number of realizations. For $J > J_c$,

$$|c_R| \sim \frac{1}{\pi}\sqrt{\alpha(J_c)\beta(J_c)(J - J_c) + \gamma\beta(J_c)\xi_0}$$

the average

$$\overline{c} = \frac{1}{N}\sum_{R=1}^{N}|c_R| = \frac{1}{2\pi}\int_{-1}^{1}(\alpha\beta(J - J_c) + \gamma\beta\xi)^{1/2}d\xi \sim (J - J_c^*)^{3/2}$$

where the new critical field is $J_c^* = J_c - \frac{\gamma}{\alpha}$.

As $\nu \to 0$, only fronts traveling in one direction remain, same as for the continuous limit, a reaction-convection-diffusion equation:

$$\frac{dE}{dt} + v(E)E_x - D(E)E_{xx} = J - v(E).$$

4.2 Hyperbolic and kinetic models for the Gunn effect

When we add boundaries and wish to describe the so-called Gunn effect, that is, generation of successive electric pulses at one end which travel and die at the other end, triggering the creation of a new one [5]. This phenomenon is captured at a macroscopic level by the system

$$\begin{aligned}
\frac{\partial^2 E}{\partial x\partial t} + A\frac{\partial E}{\partial t} + B\frac{\partial E}{\partial x} + C\frac{\partial J}{\partial t} + D = 0, &\qquad x \in (0, L),\ t > 0,\\
E(x, 0) = 0, &\qquad x \in (0, L),\\
E(0, t) = \rho J(t), &\qquad t \geqq 0,\\
\int_0^L E(x, t)dx = \phi, &\qquad t \geqq 0,
\end{aligned}$$

where ρ, ϕ, L are positive and A, B, C, D are bounded functions, A and B positive, while C is negative. $E(x, t)$ represents the electric field and $J(t)$ the current, while ϕ is the voltage.

More detailed microscopic models for this phenomena lead to kinetic Boltzmann equations for semiconductors [9, 31] for the carrier density $f(x, k, t)$ such as

$$\begin{aligned}
&\partial_t f + \frac{\Delta l}{2\hbar v_M}\sin(k)\partial_x f + \frac{\tau_e}{\eta}F\partial_k f = \\
&\quad \frac{1}{\eta}\left[f^{FDa}(k; \mu(n)) - \left(1 + \frac{\nu_{imp}}{2\nu_{en}}\right)f + \frac{\nu_{imp}}{2\nu_{en}}f(x, -k, t)\right],
\end{aligned}$$

$$\partial_x^2 V = \partial_x F = n - 1$$

$$n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x,k,t)\, dk = \frac{1}{2\pi} \int_{-\pi}^{\pi} f^{FDa}(k;\mu(n))\, dk$$

$$f^{FDa}(k;\mu) = \alpha \ln\left[1 + \exp\left(\mu - \delta + \delta\cos(k)\right)\right]$$

$$\eta = \frac{v_M}{\nu_{en} x_0} \qquad \delta = \frac{\Delta}{2k_B T}.$$

The boundary conditions are, for $x = 0$:

$$f^{+} = \beta F - \frac{f^{(0)}}{\int_0^{\pi} \sin(k)\, f^{(0)}\, dk} \int_{-\pi}^{0} \sin(k)\, f^{-}\, dk$$

with

$$\beta = \frac{2\pi\hbar\sigma F_M}{e\Delta N_D}$$

and for $x = L/x_0$:

$$f^{-} = \frac{f^{(0)}}{(1/(2\pi)) \int_{-\pi}^{0} f^{(0)}\, dk} \left(1 - \frac{1}{2\pi} \int_0^{\pi} f^{+}\, dk\right)$$

The boundary conditions for the electric potential V are

$$V(0,t) = 0, \quad V(L,t) = \phi_L \sim \frac{\phi}{F_M} \frac{L}{x_0}.$$

The initial condition is

$$f^{(0)}(k;n) = \sum_{j=-\infty}^{\infty} \exp(\imath jk)\, \frac{1 - \imath jF/\tau_e}{1 + j^2 (F)^2} f_j^{FD}(n)$$

$$f_j^{FD}(n) = \frac{1}{\pi} \int_0^{\pi} f^{FD}(k;\mu(n))\, \cos(jk)\, dk$$

with $x \in [0, L = L/x_0]$ and f periodic in k with period 2π. The average energy E is defined as

$$E = \frac{E}{k_B T} = \frac{\int_{-\pi/l}^{\pi/l} \varepsilon(k) f(x,k,t)\, dk}{k_B T \int_{-\pi/l}^{\pi/l} f(x,k,t)\, dk} = \delta \frac{\int_{-\pi}^{\pi} (1 - \cos k)\, f(x,k,t)\, dk}{\int_{-\pi}^{\pi} f(x,k,t)\, dk}.$$

This model implements a BGK approximation of the collision kernel in the equation for the carrier density. The full model involves a nonlocal collision kernel and equations for different types of carriers [9].

5 Bubble and particle formation

5.1 Homogeneous nucleation of particles

Homogeneous nucleation occurs in many examples of first order phase transitions such as condensation of liquid droplets from a supersaturated vapor, glass-to-crystal transformations, crystal nucleation in undercooled liquids, and in polymers, colloidal crystallization, growth of spherical aggregates beyond the critical micelle concentration (CMC), and the segregation by coarsening of binary alloys quenched into the miscibility gap.

Consider a model nucleation in a lattice in which there are many more binding sites, M, than particles, N. We shall consider the thermodynamic limit, $N \to \infty$, with fixed particle density per site, $\rho = N/M$. Let p_k be the number of clusters with k particles or, in short, k clusters, and let $\rho_k = p_k/M$ be the density of k clusters. Particle conservation implies that the total particle density ρ is constant

$$\sum_{k=1}^{\infty} k\rho_k = \rho.$$

In the Becker-Döring kinetic theory of nucleation, a k cluster can grow or decay by capturing or shedding one monomer at a time. Then the evolution with time is given by

$$\rho_k' = j_{k-1} - j_k, \quad k \geqq 2,$$
$$j_k = d_k(e_{(\epsilon_{k+1}-\epsilon_k)/(K_B T)}\rho_1\rho_k - \rho_{k+1}).$$

The monomer density ρ_1 can be obtained from the conservation identity that relates it to the other cluster densities. Different eras in the process of cluster formation can be analyzed by adequate asymptotic methods [17, 21].

5.2 Heterogeneous nucleation

Heterogeneous nucleation happens at preferential sites where irregularities are located.

5.2.1 Bubble formation in radioactive waste

The formation and growth of helium bubbles due to self-irradiation in plutonium has been modeled by discrete kinetic equations for the number densities of bubbles having k atoms. This is an important phenomenon which occurs in radioactive waste and may end up damaging containers resulting in radioactive pollution of the environment. As an alloy ages, there is an initial transient stage during which self-irradiation produces dislocation loops that tend to saturate within approximately two years. The alpha particles created during irradiation become helium atoms. These atoms come to rest at unfilled vacancies generated during their slowing-down process, before they are captured at existing helium bubbles. A helium atom diffuses through the lattice until it finds another helium atom thereby forming a stable dimer or until it finds a helium bubble (a stable cluster with k atoms or, in short, a k-cluster), which absorbes it. Helium bubbles are attached to lattice defects, do not move and do not shed helium atoms because the binding energies of helium to any cluster are extremely high.

We denote by $\rho_k(t)$ the number density of k clusters having effective radii a_k (when the centre of a monomer comes within distance a_k of the cluster centre, it is absorbed). $\rho_1(t)$ is the number of monomers per unit volume, D is the diffusion coefficient and $g(t)$ is the number of monomers created per unit volume and per unit time. The following kinetic model describes the process

$$\rho_k' = 4\pi D\rho_1 a_{k-1}\rho_{k-1} - 4\pi D\rho_1 a_k\rho_k, \quad k \geqq 3,$$
$$\rho_2' = 8\pi D\rho_1^2 a_1 - 4\pi D\rho_1 a_2\rho_2,$$
$$\rho_1 + \sum_{k=2}^{\infty} k\rho_k = \int_0^t g(s)ds$$

Asymptotic studies [22] show that this system generates a wave profile describing the evolution of the number of clusters of different sizes with time.

5.2.2 Deposition of vapour and particles

Heterogeneous condensation of vapours mixed with a carrier gas in the stagnation point boundary layer flow near a cold wall is considered in the presence of solid particles much larger than the mean free path of vapour particles. The supersaturated vapour condenses on the particles by diffusion, and particles and droplets are thermophoretically attracted to the wall.

Consider a dilute vapour of number density $c(x)$ in a carrier gas that contains a small amount of solid single-size particles. The mass fraction of vapour and of solid particles are sufficiently small with respect to the mass fraction of the carrier gas, so that the velocity and temperature fields (assumed to be stationary) $u(x)$ and $T(x)$ are not affected by the condensation and deposition processes. The solid particles can act as condensation sites for the vapour. Let n^* be the volume of a particle divided by the molecular volume of condensed vapour, so that a solid particle is equivalent to n^* molecules of vapour. Then a droplet of liquid coating on a solid particle is equivalent to $n(x)$ vapour molecules, in the sense that n equals the volume of a droplet (particle plus condensed vapour) divided by the molecular volume of condensed vapour. Thus, the number of liquid molecules coating a given solid particle is $n(x) - n^*$. Let $\rho(x)$ be the number density of droplets, so that $\rho(x)[n(x) - n^*]$ is the number density of the condensate.

Let us fix a flow geometry, a stagnation point flow near a wall. The equations for $u(x)$, $n(x)$, $T(x)$ and $c(x)$ are [30]

$$
\begin{aligned}
u''' + uu'' + 1 - (u')^2 = 0, \quad x > 0,\\
u(0) = u'(0) = 0,\ u'(\infty) = 1,\\
T'' + Pr\, uT' = 0, \quad x > 0,\\
T(0) = T_w,\ T(\infty) = 1,\\
\left(u + \alpha \frac{T'}{T}\right) \rho' = -\alpha\rho \left(\frac{T'}{T}\right)', \quad x > 0,\\
\rho(\infty) = 1,\\
\left(u + \alpha \frac{T'}{T}\right) n' = -N n^{1/3}(c - c_e) \quad x_* > x > 0,\\
n(x_*) = 1,\\
c_e(x) = \frac{T_d}{T(x)} exp\left[\frac{1}{\epsilon}\left(\frac{1}{T_d} - \frac{1}{T(x)}\right)\right],\\
c'' + Sc\, uc' = R\rho n^{1/3}(c - c_e), \quad 0 < x < x_*,\\
c(0) = c_e(0),\ c(x_*) = c_e(x_*),\\
c'' + Sc\, uc' = 0, \quad x > x_*,\\
c(x_*) = c_e(x_*),\ c'(x_*^-) = c'(x_*^+)\ c(\infty) = 1,
\end{aligned}
$$

where the point x^* comes with the solution of the free boundary problem [30].

6 Graphene defects

Graphene is a two dimensional material with promising mechanical and electronic properties. Its lattice structure consists of carbon atoms forming a hexagonal lattice. Different types of defects alter the hexagonal structure, as well as the mechanic and electronic properties of the material as a consequence. Periodized discrete elasticity models can describe typical defects and their dynamics [28, 26].

Consider a planar hexagonal graphene lattice and ignore possible vertical deflections. In the continuum limit, in-plane deformations are described by the Navier equations of linear elasticity for the two-dimensional (2D) displacement vector (u, v),

$$
\begin{aligned}
\rho_2 \frac{\partial^2 u}{\partial t^2} &= (\lambda + 2\mu) \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 v}{\partial x \partial y},\\
\rho_2 \frac{\partial^2 v}{\partial t^2} &= \mu \frac{\partial^2 v}{\partial x^2} + (\lambda + 2\mu) \frac{\partial^2 v}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 u}{\partial x \partial y},
\end{aligned}
$$

where ρ_2 is the 2D mass density and λ and μ are the 2D Lamé coefficients ($\lambda = C_{12}$, $\mu = C_{66}$, $\lambda + 2\mu = C_{11}$).

At lattice level, we obtain a discrete elasticity model for the atom dynamics as follows. We consider a point A in the hexagonal lattice with coordinates (x, y). Its 9 (3+6) closest neighbours have coordinates

$$n_1 = \left(x - \frac{a}{2}, y - \frac{a}{2\sqrt{3}}\right), \; n_2 = \left(x + \frac{a}{2}, y - \frac{a}{2\sqrt{3}}\right), \; n_3 = \left(x, y + \frac{a}{\sqrt{3}}\right),$$
$$n_4 = \left(x - \frac{a}{2}, y - \frac{a\sqrt{3}}{2}\right), \; n_5 = \left(x + \frac{a}{2}, y - \frac{a\sqrt{3}}{2}\right), \; n_6 = (x - a, y),$$
$$n_7 = (x + a, y), \; n_8 = \left(x - \frac{a}{2}, y + \frac{a\sqrt{3}}{2}\right), \; n_9 = \left(x + \frac{a}{2}, y + \frac{a\sqrt{3}}{2}\right).$$

Let us define the following operators acting on functions of the coordinates (x, y) of node A:

$$\begin{aligned} Tu &= [u(n_1) - u(A)] + [u(n_2) - u(A)] + [u(n_3) - u(A)], \\ Hu &= [u(n_6) - u(A)] + [u(n_7) - u(A)], \\ D_1 u &= [u(n_4) - u(A)] + [u(n_9) - u(A)], \\ D_2 u &= [u(n_5) - u(A)] + [u(n_8) - u(A)], \end{aligned}$$

Taylor expansions of these finite difference combinations about (x, y) yield

$$\begin{aligned} Tu &\sim \left(\partial_x^2 u + \partial_y^2 u\right) \frac{a^2}{4}, \\ Hu &\sim (\partial_x^2 u)\, a^2, \\ D_1 u &\sim \left(\frac{1}{4}\,\partial_x^2 u + \frac{\sqrt{3}}{2}\,\partial_x \partial_y u + \frac{3}{4}\,\partial_y^2 u\right) a^2, \\ D_2 u &\sim \left(\frac{1}{4}\,\partial_x^2 u - \frac{\sqrt{3}}{2}\,\partial_x \partial_y u + \frac{3}{4}\,\partial_y^2 u\right) a^2, \end{aligned}$$

as $a \to 0$. Now we replace in the motion equations Hu/a^2, $(4T - H)u/a^2$ and $(D_1 - D_2)u/(\sqrt{3}a^2)$ instead of $\partial_x^2 u$, $\partial_y^2 u$ and $\partial_x \partial_y u$, respectively, with similar substitutions for the derivatives of v, thereby obtaining the following equations at each point of the lattice:

$$\begin{aligned} \rho_2 a^2 \frac{\partial^2 u}{\partial t^2} &= 4\mu\, Tu + (\lambda + \mu)\, Hu + \frac{\lambda + \mu}{\sqrt{3}}\, (D_1 - D_2) v, \\ \rho_2 a^2 \frac{\partial^2 v}{\partial t^2} &= 4(\lambda + 2\mu)\, Tv - (\lambda + \mu) Hv + \frac{\lambda + \mu}{\sqrt{3}}\, (D_1 - D_2) u. \end{aligned}$$

The isotropic Navier equations have singular solutions such as

$$\begin{aligned} u &= \frac{a}{2\pi} \left[\tan^{-1}\left(\frac{y}{x}\right) + \frac{xy}{2(1-\nu)(x^2+y^2)}\right], \\ v &= \frac{a}{2\pi} \left[-\frac{1-2\nu}{4(1-\nu)}\, \ln\left(\frac{x^2+y^2}{b^2}\right) + \frac{y^2}{2(1-\nu)(x^2+y^2)}\right], \end{aligned}$$

where $\nu = \lambda/[2(\lambda+\mu)]$ for any a. These solutions represent edge dislocations. We choose (x_0, y_0) different from a lattice point and solve a damped version of the discrete Navier equations

$$\begin{aligned}
\rho_2 a^2 \frac{\partial^2 u}{\partial t^2} + \gamma \frac{\partial u}{\partial t} &= 4\mu\, Tu + (\lambda+\mu)\, Hu + \frac{\lambda+\mu}{\sqrt{3}}\, (D_1 - D_2) v, \\
\rho_2 a^2 \frac{\partial^2 v}{\partial t^2} + \gamma \frac{\partial v}{\partial t} &= 4(\lambda+2\mu)\, Tv - (\lambda+\mu) Hv + \frac{\lambda+\mu}{\sqrt{3}}\, (D_1 - D_2) u,
\end{aligned}$$

with $\gamma > 0$. Starting from $(u(x-x_0, y-y_0), v(x-x_0, y-y_0))$, the system relaxes as time grows to a stationary solution that contains a typical heptagon-pentagon defect (sometimes octagons). These are standard defects observed in graphene.

To allow for motion and interaction of these defects taking into account the lattice directions we change coordinates from cartesian coordinates to the primitive lattice coordinates and periodize the differences along them with the lattice constant periodicity [28, 26]. Heptagon-pentagon pairs differently oriented interact through their elastic far fields, attracting and repelling, to form known defects, such as unstable Stone-Wales and different types of dipoles and loops.

7 Imaging of structures

In many situations we need to extract information on the inner structure of a medium from external indirect observations. Technology has provided many tools for different purposes: magnetic resonance, tomography, ultrasound, radar, seismic imaging... All of them are based on emitting some kind of wave which interacts with the medium under study, and is then measured at a set of receptors. Knowing the data recorded at the receptors and the emitted waves, we wish to reconstruct the internal geometry and/or material properties of the medium. Topological derivative based methods have arisen as a powerful tool to obtain information on objects from scattered data.

7.1 Acoustic waves

Let us consider a medium where a number of objects are buried. To simplify, we take the surrounding medium to be $\Omega_e := \mathbb{R}^2 \setminus \overline{\Omega}_i$, $\Omega_i \subset \mathbb{R}^2$ being the obstacle. Ω_i is an open bounded set with smooth boundary $\Gamma := \partial\Omega_i$ but has no assumed connectivity. There may be an unknown number of isolated components: $\Omega_i = \cup_{j=1}^{d} \Omega_{i,j}$ with $\Omega_{i,j}$ open connected bounded sets satisfying $\overline{\Omega}_{i,l} \cap \overline{\Omega}_{i,j} = \emptyset$ for $l \neq j$.

This configuration is illuminated by a plane wave $u_{inc}(\mathbf{x}) = \exp(\imath\, \kappa^0\, \mathbf{x} \cdot \mathbf{d})$ with wave number κ^0 and propagation direction $\mathbf{d}, |\mathbf{d}| = 1$. The incident wave interacts with the medium and the obstacles, generating a scattered wave and a transmitted wave. The total wave field is measured at detector locations placed on Γ_{meas}, far enough from the scatterers. Γ_{meas} may be a circle enclosing the obstacles in simple tests or a number of sites where receptors are located in more realistic reconstructions. In real experiments, the total field is known on the set of receptors Γ_{meas} for several incident directions $\mathbf{d}^j$.

The interaction between the scatterers, the medium and the incident radiation is described by the following scalar transmission model. The total scalar wave field $u = u_{inc} + u_{sc}$ in Ω_e and the transmitted scalar wave field $u = u_{tr}$ in Ω_i satisfy

$$\left| \begin{array}{ll} \nabla \cdot (\alpha_e \nabla u) + \lambda_e^2 u = 0, & \text{in } \Omega_e, \\ \nabla \cdot (\alpha_i \nabla u) + \lambda_i^2 u = 0, & \text{in } \Omega_i, \\ u^- - u^+ = 0, & \text{on } \Gamma, \\ \alpha_i \partial_{\mathbf{n}} u^- - \alpha_e \partial_{\mathbf{n}} u^+ = 0, & \text{on } \Gamma, \\ \lim_{r \to \infty} r^{1/2} \big(\partial_r (u - u_{inc}) - \imath \kappa^0 (u - u_{inc}) \big) = 0, & r = |\mathbf{x}|, \end{array} \right.$$

with real parameters

$$\lambda_e(\mathbf{x}) \geq \lambda_e^1 > 0, \quad \lambda_i(\mathbf{x}) \geq \lambda_i^1 > 0, \quad \alpha_e(\mathbf{x}) \geq \alpha_e^1 > 0, \quad \alpha_i(\mathbf{x}) \geq \alpha_i^1 > 0.$$

The normal vector $\mathbf{n}$ points inside Ω_i. u^+ and u^- denote the limits of u from the exterior and interior of Ω_i respectively. $\partial_{\mathbf{n}}$ and ∂_r stand for normal and radial derivatives.

Knowing the values of the field u at a number of receptors, $u_{\rm meas}$, for different incident waves we wish to obtain information on the objects buried in the medium. We can look for domains Ω_i which minimize an error in some sense. This leads to a constrained optimization problem: minimize

$$J(\mathbb{R}^2 \setminus \overline{\Omega}_i) := \frac{1}{2} \sum_{j=1}^{M} \int_{\Gamma_{meas}} |u^j - u^j_{\rm meas}|^2 dl,$$

u^j being the solutions of M forward transmission problems with incident waves $u^j_{inc}(\mathbf{x}) = \exp(\imath \kappa^0 \mathbf{x} \cdot \mathbf{d}^j)$. This functional depends on the design variable Ω_i through the transmission problems, which act as constraints.

The topological derivative of this cost functional helps to locate the objects.The topological derivative of the shape functional $\mathcal{J}(\mathcal{R})$ is defined as

$$D_T(\mathbf{x}, \mathcal{R}) := \lim_{\varepsilon \to 0} \frac{\mathcal{J}(\mathcal{R}_\varepsilon) - \mathcal{J}(\mathcal{R})}{\mathcal{V}(\varepsilon)}, \qquad \mathbf{x} \in \mathcal{R},$$

where $\mathcal{V}(\varepsilon)$ is minus the volume of the ball. In our case, $\mathcal{V}(\varepsilon) = -\pi\varepsilon^2$. Asymptotic expansions provide a result easier to implement [25, 27]: The topological derivative of the cost functional in $\mathcal{R} = \mathbb{R}^2 \setminus \overline{\Omega}$ is given by

$$D_T(\mathbf{x}, \mathbb{R}^2 \setminus \overline{\Omega}) = \sum_{j=1}^{M} \mathrm{Re} \Bigg[\frac{2(\alpha_e(\mathbf{x}) - \alpha_i(\mathbf{x}))}{1 + \frac{\alpha_i(\mathbf{x})}{\alpha_e(\mathbf{x})}} \nabla u^j(\mathbf{x}) \nabla \overline{p}^j(\mathbf{x}) + (\lambda_i^2(\mathbf{x}) - \lambda_e^2(\mathbf{x}))\, u^j(\mathbf{x}) \overline{p}^j(\mathbf{x}) \Bigg],$$

for any $\mathbf{x} \in \mathbb{R}^2 \setminus \overline{\Omega}$ not belonging to the singularity curves of the parameters. The forward field u^j solves the forward transmission problems with the j-th incident wave and $\Omega_i = \Omega$. The adjoint field p^j solves

$$\left| \begin{array}{ll} \nabla \cdot (\alpha_e \nabla p^j) + \lambda_e^2 p = (u^j_{meas} - u^j)\, \delta_{\Gamma_{meas}}, & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}_i\ , \\ \nabla \cdot (\alpha_i \nabla p^j) + \lambda_i^2 p^j = 0, & \text{in } \Omega_i, \\ (p^j)^- - (p^j)^+ = 0, & \text{on } \partial\Omega_i, \\ \alpha_i \partial_{\mathbf{n}} (p^j)^- - \alpha_e \partial_{\mathbf{n}} (p^j)^+ = 0, & \text{on } \partial\Omega_i, \\ \lim_{r\to\infty} r^{1/2} \left(\partial_r p^j + \imath \kappa^0 p^j \right) = 0, & \end{array} \right.$$

with $\Omega_i = \Omega$. Here, $\delta_{\Gamma_{meas}}$ is the Dirac delta function defined on Γ_{meas}. Visualizing the topological derivative field for $\Omega_i = \Omega = \emptyset$ we find information on the objects. An iterative procedure allows us to improve it [27].

7.2 Thermal waves

The previous description corresponds to an imaging problem with time harmonic acoustic waves. A similar strategy can be applied to time dependent thermal waves [29], which solve transmission heat problems

$$\left\{ \begin{array}{ll} U_t - \kappa_e \Delta U = 0, & \text{in } \mathbb{R}^N \setminus \overline{\Omega_i} \times (0,\infty), \\ U_t - \alpha_i \kappa_i \Delta U = 0, & \text{in } \Omega_i \times (0,\infty), \\ U^- - U^+ = U_{\rm inc}, & \text{on } \partial\Omega_i \times (0,\infty), \\ \alpha_i \frac{\partial}{\partial \mathbf{n}} U^- - \frac{\partial}{\partial \mathbf{n}} U^+ = \frac{\partial}{\partial \mathbf{n}} U_{\rm inc}, & \text{on } \partial\Omega_i \times (0,\infty), \\ U(\,\cdot\,,0) = 0, & \text{in } \mathbb{R}^N, \end{array} \right.$$

Topological derivative methods allow us to approximate solutions of the inverse problem for such waves [29].

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