# Supplemental Material: Thermal fluctuations of dislocations reveal the interplay between their core energy and long-range elasticity

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## 1 Elastic energy of a perturbed dislocations

We consider an isolated dislocation described by the non-singular theory of Cai et al. [1]. This theory presents the advantage of avoiding the singular behavior of the stress and strain fields at the dislocation core encountered in the classical theory of dislocations [2]. The centerpiece of the non-singular theory is to spread isotropically the Burgers vector of the dislocation over a characteristic distance a, hereafter referred to as the core parameter. In the framework of linear elasticity, the self-energy of such a dislocation is given by<sup>1</sup>:

$$W = -\frac{\mu}{16\pi} \int_C \int_C \partial_k \partial_k R_a b_i b_j dx_i dx'_j - \frac{\mu}{8\pi(1-\nu)} \int_C \int_C \partial_i \partial_j R_a b_i b_j dx_k dx'_k$$
(1)  
+ 
$$\frac{\mu}{8\pi(1-\nu)} \left[ \int_C \int_C \partial_k \partial_k R_a b_i b_j dx_j dx'_j - \nu \int_C \int_C \partial_k \partial_k R_a b_i b'_j dx_j dx'_i \right]$$

where **b** is the Burgers vector of the dislocation,  $\mu$  and  $\nu$  respectively denote the shear modulus and Poisson ration of the material,  $R_a = \sqrt{a^2 + (x - x')^2 + (y - y')^2 + (z - z')^2}$  and the integrals run along the dislocation line.

In the following, we will consider the case of an infinitely long dislocation along the x direction, gliding in the (x, y) plane. We restrict ourselves to the case of a glissile dislocation with a Burgers vector  $\boldsymbol{b} = [b_s, b_e, 0]$ . The self-energy of such a dislocation can be decomposed in the following way:

<sup>&</sup>lt;sup>1</sup>Notice the difference of a factor 2 in comparison with Eq. (31) of Ref. [1] which actually describes the interaction energy of a loop with itself (i.e. twice its self-energy)

$$W = W_{screw}(b_s^2) + W_{edge}(b_e^2) + W_{cross}(b_s \cdot b_e)$$
<sup>(2)</sup>

with

$$W_{screw} = \frac{\mu b_s^2}{16\pi} \int_C \int_C \left(\frac{2}{R_a} + \frac{a^2}{R_a^3}\right) dl_x dl'_x + \frac{\mu b_s^2}{8\pi (1-\nu)} \int_C \int_C \left(\frac{2}{R_a} - \frac{(y-y')^2}{R_a^3}\right) dl_y dl'_y \qquad (3)$$
$$- \frac{\mu b_s^2}{8\pi (1-\nu)} \int_C \int_C \left(\frac{1}{R_a} - \frac{(x-x')^2}{R_a}\right) dl_x dl'_x,$$

$$W_{edge} = \frac{\mu b_e^2}{16\pi} \int_C \int_C \left(\frac{2}{R_a} + \frac{a^2}{R_a^3}\right) dl_y dl'_y + \frac{\mu b_e^2}{8\pi(1-\nu)} \int_C \int_C \left(\frac{2}{R_a} - \frac{(x-x')^2}{R_a^3}\right) dl_x dl'_x \quad (4)$$
$$-\frac{\mu b_e^2}{8\pi(1-\nu)} \int_C \int_C \left(\frac{1}{R_a} - \frac{(y-y')^2}{R_a^3}\right) dl_y dl'_y$$

and

$$W_{cross} = \frac{\mu b_s b_e}{4\pi (1-\nu)} \left[ \int_C \int_C \left( \frac{(x-x')(y-y')}{R_a^3} \right) dl_x dl'_x + \int_C \int_C \left( \frac{(x-x')(y-y')}{R_a^3} \right) dl_y dl'_y \right] - \frac{\mu b_s b_e}{4\pi} \frac{1+\nu}{1-\nu} \int_C \int_C \left( \frac{1}{R_a} + \frac{a^2}{R_a^3} \right) dl_x dl'_y$$
(5)

We now assume that the position of the dislocation line can be described by a function h(x), periodic in x with a periodicity L. Then, we have  $dl_x = dx$  and  $dl_y = h'(x)dx$  and we note  $w(h) = w_{screw}(h) + w_{edge}(h) + w_{cross}(h)$  the energy of a portion L of the dislocation. In addition, we are interested in the energy difference E(h) over a distance L between a perturbed state (described by h(x)) and an unperturbed state of the dislocation. In the following, we will also consider that the function h(x) varies slowly with x to simplify further the expression of the energy. As for Eq. (2), we can decompose E(h) in the following way:

$$E(h) = (w_{screw}(h) - w_{screw}(\mathbf{0})) + (w_{edge}(h) - w_{edge}(\mathbf{0})) + (w_{cross}(h) - w_{cross}(\mathbf{0}))$$
  
=  $E_{screw}(h)$  +  $E_{edge}(h)$  +  $E_{cross}(h)$  (6)

In the following, we will successively focus on these three contributions to obtain the energy of an arbitrary perturbation h(x).

#### **1.1 Screw contribution** $E_{screw}(h)$

For a portion L of the infinite dislocation, the energy  $E_{screw}(h)$  is expressed as:

$$E_{screw}(h) = \frac{\mu b_s^2}{8\pi} \int_0^L \int_{-\infty}^{+\infty} \left(\frac{1}{\tilde{R}_a} - \frac{1}{\bar{R}_a}\right) dx dx' - \frac{\mu b_s^2}{16\pi} \frac{1+\nu}{1-\nu} \int_0^L \int_{-\infty}^{+\infty} \left(\frac{a^2}{\tilde{R}_a^3} - \frac{a^2}{\bar{R}_a^3}\right) dx dx'$$
(7)  
+  $\frac{\mu b_s^2}{8\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{h'(x)h'(x')}{\tilde{R}_a} dx dx' - \frac{\mu b_s^2}{8\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(h(x) - h(x'))^2}{\tilde{R}_a^3} dx dx'$ (7)  
+  $\frac{\mu b^2}{8\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{h'(x)h'(x')\left((x-x')^2 + a^2\right)}{\tilde{R}_a^3} dx dx'$ 

where  $\tilde{R}_a = \sqrt{a^2 + (x - x')^2 + (h(x) - h(x'))^2}$  and  $\bar{R}_a = \sqrt{a^2 + (x - x')^2}$  are respectively related to the perturbed and unperturbed states.

We now consider that the variations of h(x) are small, i.e. that  $\max_x |h'(x)| = h'_{max} \ll 1$  and consequently  $\left|\frac{h(x)-h(x')}{x-x'}\right| \ll 1$  for any x and x'. In this limit, the integrals of Eq. (7) can be simplified using Taylor expansions. For example, the first integral of Eq. (7) becomes:

$$\int_{0}^{L} \int_{-\infty}^{+\infty} \left(\frac{1}{\bar{R}_{a}} - \frac{1}{\bar{R}_{a}}\right) dx dx' = -\frac{1}{2} \int_{0}^{L} \int_{-\infty}^{+\infty} \frac{(h(x) - h(x'))^{2}}{(a^{2} + (x - x')^{2})^{3/2}} dx dx' + \mathcal{O}(h_{max}'^{4}) \tag{8}$$

Performing similar Taylor expansions for the other integrands and keeping only the lowest order terms in  $h'_{max}$  yields:

$$E_{screw}(h) = \frac{\mu b_s^2}{4\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{h'(x)h'(x')}{\sqrt{a^2 + (x-x')^2}} dx' dx - \frac{\mu b_s^2 (3-\nu)}{16\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(h(x) - h(x'))^2}{(a^2 + (x-x')^2)^{3/2}} dx' dx + \frac{3\mu b_s^2 (1+\nu)}{32\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{a^2 (h(x) - h(x'))^2}{(a^2 + (x-x')^2)^{5/2}} dx' dx + \mathcal{O}(h_{max}'^4)$$
(9)

For simplicity, the asymptotic notation  $\mathcal{O}(h_{max}^{\prime 4})$  is omitted in the following.

Since h(x) is a real *L*-perioric function, it can be expressed as a Fourier series:

$$h(x) = \sum_{n=-N_{max}}^{N_{max}} C_n e^{ik_n x}$$

$$\tag{10}$$

where  $k_n = 2\pi n/L$  are wave numbers and the complex Fourier coefficients satisfy  $C_{-n} = C_n^*$ because h(x) is a real function. In practice, the number of modes  $N_{max}$  can be chosen in relation with a small atomic length-scale (e.g.  $N_{max} = int(L/b)$ ).

The first integral of Eq. (9) can be rewritten as

$$I_{1}(h) = \int_{0}^{L} \int_{-\infty}^{+\infty} -\frac{(\sum_{n} k_{n} C_{n} e^{ik_{n}x})(\sum_{m} k_{m} C_{m} e^{ik_{m}x'})}{\sqrt{a^{2} + (x - x')^{2}}} dx' dx$$
  
$$= -\sum_{n} \sum_{m} C_{n} C_{m} k_{n} k_{m} \int_{0}^{L} \int_{-\infty}^{+\infty} \frac{e^{ik_{n}x} e^{ik_{m}x'}}{\sqrt{a^{2} + (x - x')^{2}}} dx dx'$$
  
$$= -\sum_{n} \sum_{m} C_{n} C_{m} k_{n} k_{m} \int_{0}^{L} e^{i(k_{n} + k_{m})x} dx \int_{-\infty}^{+\infty} \frac{e^{iak_{m}u}}{\sqrt{1 + u^{2}}} du$$

with u = (x - x')/a. Here, we recognize the expression of the modified Bessel function of second kind of order 0 defined as:

$$K_0(z) = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{e^{izu}}{\sqrt{1+u^2}} du,$$
(11)

In addition,  $\int_0^L e^{i(k_n+k_m)} = 0$  for  $m \neq -n$  and = L otherwise. Therefore, we can directly write

$$I_1(h) = \sum_{n=1}^{N_{max}} 4|C_n|^2 k_n^2 L K_0(ak_n).$$
(12)

Similarly, the other integrals of Eq. (9) can be expressed as functions of modified Bessel functions of order 1 and 2 respectively denoted  $K_1$  and  $K_2$ :

$$I_2(h) = \int_0^L \int_{-\infty}^{+\infty} \frac{(h_n(x) - h_n(x'))^2}{(a^2 + (x - x'))^{3/2}} dx' dx = \frac{8|C_n|^2 L}{a^2} \left(1 - ak_n K_1(ak_n)\right)$$
(13)

$$I_3(h) = \int_0^L \int_{-\infty}^{+\infty} \frac{a^2 (h_n(x) - h_n(x'))^2}{(a^2 + (x - x'))^{5/2}} dx' dx = \frac{8|C_n|^2 L}{3a^2} \left(2 - (ak_n)^2 K_2(ak_n)\right).$$
(14)

Therefore, the screw contribution of the perturbation h(x) can be expressed in the following compact form:

$$E_{screw}(h) = \sum_{n=1}^{N_{max}} \frac{\mu b_s^2 |C_n|^2 L}{2\pi (1-\nu) a^2} \Big( 2a^2 k_n^2 K_0(ak_n) - (3-\nu) \left(1 - ak_n K_1(ak_n)\right) + \frac{1+\nu}{2} (2 - a^2 k_n^2 K_2(ak_n)) \Big)$$
(15)

#### **1.2 Edge contribution** $E_{edge}(h)$

We now focus on the edge contribution of Eq. (6). For a portion L of the infinite dislocation, the term  $E_{edge}(h)$  can be written as:

$$E_{edge}(h) = \frac{\mu b_e^2}{4\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \left(\frac{1}{\tilde{R}_a} - \frac{1}{\bar{R}_a}\right) dx dx' + \frac{\mu b_e^2}{8\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \left(\frac{a^2}{\tilde{R}_a^3} - \frac{a^2}{\bar{R}_a^3}\right) dx dx' + \frac{\mu b_e^2}{8\pi} \int_0^L \int_{-\infty}^{+\infty} \frac{h'(x)h'(x')}{\tilde{R}_a} dx dx' + \frac{\mu b_e^2}{16\pi} \int_0^L \int_{-\infty}^{+\infty} \frac{a^2 h'(x)h'(x')}{\tilde{R}_a^3} dx dx'$$
(16)  
$$- \frac{\mu b_e^2}{8\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \left(a^2 + (x-x')^2\right) \left(\frac{1}{\tilde{R}_a} - \frac{1}{\bar{R}_a}\right) dx dx' - \frac{\mu b_e^2}{8\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(a^2 + (x-x')^2)h'(x)h'(x')}{\tilde{R}_a^3} dx dx'$$

with  $\tilde{R}_a = \sqrt{a^2 + (x - x')^2 + (h(x) - h(x'))^2}$  and  $\bar{R}_a = \sqrt{a^2 + (x - x')^2}$ 

We now consider that the variations of h(x) are small. As in the previous section, we perform Taylor expansions of the different integrands and reorganize the different terms to obtain

$$E_{edge}(h) = -\frac{\mu b_e^2}{8\pi} \frac{\nu}{1-\nu} \int_0^L \int_{-\infty}^{+\infty} \frac{h'(x)h'(x')}{\sqrt{a^2 + (x-x')^2}} dx' dx + \frac{\mu b_e^2}{16\pi} \int_0^L \int_{-\infty}^{+\infty} \frac{a^2 h'(x)h'(x')}{(a^2 + (x-x')^2)^{3/2}} dx' dx + \frac{\mu b_e^2}{16\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(h(x) - h(x'))^2}{(a^2 + (x-x')^2)^{3/2}} dx' dx - \frac{3\mu b_e^2}{16\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{a^2(h(x) - h(x'))^2}{(a^2 + (x-x')^2)^{3/2}} dx' dx$$
(17)

After expanding the L-periodic function h(x) in a Fourier series as in Eq. (10), we follow the same steps as in previous section and obtain:

$$E_{edge}(h) = \sum_{n=1}^{N_{max}} \frac{\mu b_e^2 |C_n|^2 L}{2\pi (1-\nu) a^2} \Big( -\nu a^2 k_n^2 K_0(ak_n) + (1-ak_n K_1(ak_n))$$
(18)

$$+ a^{3}k_{n}^{3}\frac{1-\nu}{2}K_{1}(ak_{n}) - \left(2 - (ak_{n})^{2}K_{2}(ak_{n})\right)\right)$$
(19)

## **1.3 Cross term contribution** $E_{cross}(h)$

We now focus on the cross term of Eq. (6). For a portion L of the dislocation, the energy  $E_{cross}(h)$  can be written as:

$$E_{cross}(h) = -\frac{\mu b_s b_e}{4\pi} \frac{1+\nu}{1-\nu} \int_0^L \int_{-\infty}^{+\infty} \frac{h'(x)}{\tilde{R}_a} dx dx' - \frac{\mu b_s b_e}{4\pi} \frac{1+\nu}{1-\nu} \int_0^L \int_{-\infty}^{+\infty} \frac{a^2 h'(x')}{\tilde{R}_a^3} dx dx' \qquad (20)$$
$$+ \frac{\mu b_s b_e}{4\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(x-x')(h(x)-h(x'))}{\tilde{R}_a^3} dx dx'$$
$$+ \frac{\mu b_s b_e}{4\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(x-x')(h(x)-h(x'))h'(x)h'(x')}{\tilde{R}_a^3} dx dx'$$

where  $\tilde{R}_a = \sqrt{a^2 + (x - x')^2 + (h(x) - h(x'))^2}$ . With h(x) a slowly varying function ( $|h'_{max} \ll 1$ ), this expression can be simplified to the first order to yield:

$$E_{cross}(h) = -\frac{\mu b_s b_e}{4\pi} \frac{1+\nu}{1-\nu} \int_0^L \int_{-\infty}^{+\infty} \frac{h'(x')}{\sqrt{a^2 + (x-x')^2}} dx dx' - \frac{\mu b_s b_e}{8\pi (1-\nu)} \frac{1+\nu}{1-\nu} \int_0^L \int_{-\infty}^{+\infty} \frac{a^2 h'(x')}{(a^2 + (x-x')^2)^{3/2}} dx dx' + \frac{\mu b_s b_e}{2\pi (1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(x-x')(h(x) - h(x'))}{(a^2 + (x-x')^2)^{3/2}} dx dx'$$
(21)

Writing h(x) as a Fourier series as in Eq. (10), the first integral can be written as

$$I_{1}(h) = \int_{0}^{L} \int_{-\infty}^{+\infty} -\frac{\sum_{n} iC_{n}k_{n}e^{ik_{n}x'}}{\sqrt{a^{2} + (x - x')^{2}}} dx dx'$$
  
$$= -\sum_{n=-N_{max}}^{N_{max}} iC_{n}k_{n} \int_{0}^{L} e^{ik_{n}x} dx \int_{-\infty}^{+\infty} \frac{e^{iak_{m}u}}{\sqrt{1 + u^{2}}} du$$
  
$$= 0$$
(22)

because  $\int_0^L e^{ik_n x} dx = 0$ . For the same reasons, the second and third integrals of Eq. (21) are also null.

Therefore, to the first order in  $h'_{max}$ , we have  $E_{cross}(h) = 0$ , and the energy of the mixed dislocation is simply expressed as the sum of its screw and edge contributions.

#### 1.4 Elastic energy and asymptotic behavior

Therefore, combining the expressions found for  $E_{screw}(h)$  and  $E_{edge}(h)$  yields a compact expression for the energy associated with a perturbation h of Fourier coefficients  $C_n$ :

$$E_{el}(h) = \sum_{n=1}^{N_{max}} \frac{\mu |C_n|^2 L}{2\pi (1-\nu) a^2} \left[ -\left(2b_s^2 (1-\nu) + b_e^2\right) + a^2 k_n^2 K_0(ak_n) \left(2b_s^2 - \nu b_e^2\right) + ak_n K_1(ak_n) \left((3-\nu)b_s^2 - b_e^2 \left(1 - \frac{a^2 k_n^2 (1-\nu)}{2}\right)\right) - a^2 k_n^2 K_2(ak_n) \left(\frac{b_s^2 (1+\nu)}{2} - b_e^2\right) \right]$$

$$(23)$$

Because the behavior of the Bessel functions are quite difficult to intuit, we can use their Taylor expansion to yield a simple expression in the limit of small  $ak_n$ , i.e. for perturbation wavelengths much larger than the core parameter:

$$K_0(ak_n) = -\gamma_e + \ln\left(\frac{2}{ak_n}\right) + \mathcal{O}(a^2k_n^2), \tag{24}$$

$$K_1(ak_n) = \frac{1}{ak_n} + \frac{ak_n}{4} \left( -1 + 2\gamma_e - 2\ln\left(\frac{2}{ak_n}\right) \right) + \mathcal{O}(a^2k_n^2),$$
(25)

$$K_2(ak_n) = \frac{2}{a^2k_n^2} - \frac{1}{2} + \mathcal{O}(a^2k_n^2),$$
(26)

where  $\gamma_e \simeq 0.5772$  is the Euler-Mascheroni constant. Therefore, the energy associated to a single sinusoidal perturbation of the form  $h(x) = A \sin(kx)$  takes the following form for  $ak \to 0$ :

$$E_{el}(h) = \frac{\mu |A|^2 k^2}{16\pi (1-\nu)} \left[ b_e^2 \frac{(1-2\nu)}{2} - b_s^2 (1-\nu) - \left( (1-2\nu)b_e^2 + (1+\nu)b_s^2 \right) \left( \ln\left(\frac{ak}{2}\right) + \gamma_e \right) \right] + \mathcal{O}(a^2 k^2)$$
(27)

This expression reveals that the leading  $k^2$  order term is affected by a  $\ln(ak/2)$  contribution, which becomes large for small values of ak, and represents the long-range elastic interactions, characteristic of the dislocation theory.

## 2 Core energy of a perturbed dislocation

In addition to the elastic energy, we also account for the contribution of the core energy, which represents the energy of the highly defected atoms in the dislocation core region. We introduce  $\gamma(\theta)$ , the core energy of the dislocation per unit length, function of the dislocation character, which is represented by the angle  $\theta$  between the dislocation line and its Burgers vector. The difference of core energy between the perturbed and the straight dislocation is written as:

$$E_{co}(h) = \int_0^L \gamma(\tilde{\theta}(x))\sqrt{1 + h'(x)^2}dx - \int_0^L \gamma(\theta)dx$$
(28)

where  $\theta(x)$  denotes the local angle between the dislocation line and the Burgers vector,  $\theta$  the average orientation of the dislocation ( $\theta = \frac{1}{L} \int_0^L \tilde{\theta}(x) dx$ ). To simplify this expression, we assume again that the variations of h(x) are small (i.e.  $|h'_{max}| \ll 1$ ) and that  $\gamma(\theta)$  is a smooth function of  $\theta$ . Using Taylor expansions and keeping only the first order terms in h'(x) yields

$$E_{co}(h) = \frac{\gamma(\theta) + \gamma''(\theta)}{2} \int_0^L h'(x)^2 dx$$
<sup>(29)</sup>

Writing h(x) as a Fourier series yields (see Eq. (10)):

$$E_{co}(h) = -\frac{\gamma(\theta) + \gamma''(\theta)}{2} \int_{0}^{L} \sum_{n=-N_{max}}^{N_{max}} \sum_{m=-N_{max}}^{N_{max}} k_n k_m C_n C_m e^{i(k_n + k_m)x} dx$$
  
=  $L\Gamma(\theta) \sum_{n=1}^{N_{max}} k_n^2 |C_n|^2$  (30)

where  $\Gamma(\theta) = \gamma(\theta) + \gamma''(\theta)$  is defined as the line tension. We find the expected  $k^2$  behavior, characteristic of short-range interactions [3, 4, 5].

### 3 Langevin dynamics

To further characterize the time-dependent behavior of the dislocations, we consider that the dislocation line is subjected to the following Langevin dynamics:

$$M\ddot{h}(x,t) + B\dot{h}(x,t) = -\frac{\delta e\left(h(x,t)\right)}{\delta h(x,t)} + \eta(x,t)$$
(31)

where M is an inertial mass per unit length associated with the dislocation line, B is the drag coefficient characteristic of the viscous motion of the dislocation. The right-hand side is the force acting on the dislocation, composed of the functional derivative of the energy per unit length denoted e(h(x,t)) and the random force  $\eta(x,t)$  satisfying the fluctuation-dissipation theorem and representing the forces coming from the thermal bath.

To compute the functional derivative  $\frac{\delta e(h(x))}{\delta h(x)}$ , we write the function h(x) of periodicity Las a Fourier series:  $h(x) = \sum_{n=-N_{max}}^{N_{max}} C_n e^{ik_n x}$ . The energy per unit length of this perturbed dislocation can be written as  $e(h) = \frac{E_{el}(h) + E_{co}(h)}{L} = \frac{1}{2} \sum_{n=1}^{N_{max}} |C_n|^2 \mathcal{K}(k_n)$  (see previous sections and Eq. (4) of the main text). To simplify the notations, we use here  $e_n = \frac{1}{2} \mathcal{K}(k_n)$ . From the chain rule, it is straightforward to show that

$$\frac{\delta e(h(x))}{\delta h(x)} = \frac{\delta e(h(x))}{\delta C_n} \frac{\delta C_n}{\delta h(x)} = \sum_{n=1}^{N_{max}} C_n^* e_n \ e^{-ik_n x}, \tag{32}$$

Considering that the Fourier coefficients  $C_n$  are time-dependent, Eq. (31) can be written as

$$\sum_{n=-N_{max}}^{+N_{max}} M_n \ddot{C}_n(t) e^{ik_n x} + \sum_{n=-N_{max}}^{+N_{max}} B_n \dot{C}_n(t) e^{ik_n x} = -\sum_{n=-N_{max}}^{+N_{max}} e_n C_n^*(t) e^{-ik_n x} + \eta(x,t)$$
(33)

where we now assume that the effective mass and drag coefficients may depend on the wavenumber n. After multiplication of Eq. (33) by  $e^{-ik_nx}$  and integration between 0 and L, we obtain independent dynamical equations on the different modes:

$$M_n \ddot{C}_n + B_n \dot{C}_n + e_n C_n = \eta_k(k_n, t) \tag{34}$$

where  $\eta_k(k_n, t)$  is an uncorrelated random process acting on the Fourier coefficients. We recognize here the equation of a noisy under-damped oscillator whose homogeneous solution (found for  $\eta_k(k_n, t) = 0$ ) is of the form:

$$C_n^{homo}(t) = C_n^0 \cos(\omega_n t + \phi_n) e^{-t/\tau_n}$$
(35)

with  $\omega_n = \sqrt{4M_n e_n - B_n^2/2M_n}$  and  $\tau_n = 2M_n/B_n$ . Following previous work [6], the influence of the random process  $\eta_k(k_n, t)$  can be averaged out by considering the ensemble average of the auto-correlation function:

$$\langle C_n(0)C_n^*(t)\rangle = \langle |C_n|^2 \rangle \cos(\omega_n t)e^{-t/\tau_n}.$$
(36)

#### 4 Dislocation core energy from molecular static simulations

Dislocation line energy and line tension can be estimated at 0K from molecular statics (MS) simulations. Consistent with our description of the dislocation fluctuations and previous works [7, 8, 9], we define the core energy as the difference between the energy of a relaxed atomistic configuration and the anisotropic elastic energy of the same dislocation arrangement computed within the non-singular formalism.

In the atomistic configurations, a dislocation dipole of a specific character is introduced using the software Babel [10]. The atomic positions are then relaxed using periodic boundary conditions, yielding the atomic energy of the relaxed configuration denoted  $E_{at}$ . As an example, Fig. 1.a shows the relaxed configuration obtained for a small cell containing a dipole of edge dislocations.

The elastic energy of the same dislocation configuration is computed based on the non-singular theory of dislocations [1]. The dislocation dipole is introduced through its equivalent eigenstrain that is smoothed in space over a distance a (see Ref. [11] for details). For a specific value of the core parameter a, the elastic fields and elastic energy  $E_{el}(\theta, a)$  are then computed with periodic boundary conditions using an efficient spectral method accounting for anisotropic elasticity [11].

Fig. 1.b displays the core energy defined as  $\gamma_a(\theta) = (E_{at}(\theta) - E_{el}(\theta, a))/2L_{\parallel}$  (accounting for the two dislocations of the cell) as a function of the atomic system size for a specific value of



Figure 1: (a) Atomistic configuration obtained after relaxation of a simulation cell containing a dipole of edge dislocations (only the defected atoms are shown). (b) Core energy obtained for different dislocation characters as a function of the size of the atomic system and for a core parameter equal to the lattice spacing a = 4.05 Å. (c) Core energy as a function of dislocation character  $\gamma_a(\theta)$  from atomistic calculations at 0 K. The line tension  $\Gamma_a$  for the edge and screw characters are shown with red squares and were obtained from local parabolic fits (shown with dash lines).

the core parameter equal to the lattice spacing a = 4.05 Å. Fig. 1.b shows that the core energy converges with the system size, as expected for dislocation core energies [7].

Repeating this operation for 14 different orientations ranging between  $0^{\circ}$  and  $90^{\circ}$ , we obtain the core energy as a function of  $\theta$ , displayed in Fig. 1.c. From these data, we can compute local second derivatives from polynomial fits (shown with dashed lines in Fig. 1.c) and deduce the line tension:

$$\Gamma_a(\theta) = \gamma_a(\theta) + \gamma_a''(\theta), \qquad (37)$$

which appears in the core contribution of Eq. (30). The result for the edge and screw dislocations are shown as red squares in Fig. 1. We highlight the importance to consider the line tension as opposed to the line energy: while the line energy of the screw dislocation is lower than for the edge character, the line tension of the screw is about three times higher than the edge due to the contribution of second derivative  $\gamma''_a(\theta)$ .

### 5 Additional results at different temperatures

In addition to the results presented in the main article, we performed MD simulations at 200 K and 400 K to assess the temperature-dependent behavior of the fluctuations. Fig. 2 shows the power spectra obtained at these temperatures. We first notice that the fits are as good as the ones presented in the main article at 300 K, showing that our analytical model is able to predict accurately the dislocation fluctuations at various temperatures.

Temperature $[K]$	$a_s$ [Å]	$\Gamma_s \left[ eV/\mathring{A} \right]$	$a_e$ [Å]	$\Gamma_e[eV/Å]$
200	3.25	0.103	5.09	0.046
300	3.34	0.114	5.60	0.053
400	3.44	0.117	6.06	0.057

Table 1: Fitted values of the core parameter and line tension at different temperatures for screw  $(a_s, \Gamma_s)$  and edge  $(a_e, \Gamma_e)$  dislocations.



Figure 2: Power spectra obtained at (a) 200 K and (b) 400 K.

Another advantage of considering various temperatures is to obtain temperature-dependent core parameters and line-tension coefficients. Tab. 1 displays these parameters obtained from the fit of Fig. 2 and shows that both the core parameter and the line tension increase with temperature. As mentioned in the main text of this article, the core parameter correlates with the dissociation distance of the dislocation, which has been shown to increase with temperature [12].

#### References

- W. Cai, A. Arsenlis, C. Weinberger, and V. Bulatov. A non-singular continuum theory of dislocations. J. Mech. Phys. Solids, 54(3):561–587, 2006.
- [2] J.P. Hirth and J. Lothe. Theory of Dislocations. McGraw-Hill, New York, 1968.
- [3] J.J. Hoyt, M. Asta, and A. Karma. Method for computing the anisotropy of the solid-liquid interfacial free energy. *Phys. Rev. Lett.*, 86(24):5530, 2001.
- [4] M. Asta, J.J. Hoyt, and A. Karma. Calculation of alloy solid-liquid interfacial free energies from atomic-scale simulations. *Phys. Rev. B*, 66(10):100101, 2002.
- [5] C. Misbah, O. Pierre-Louis, and Y. Saito. Crystal surfaces in and out of equilibrium: A modern view. *Rev. Mod. Phys.*, 82(1):981, 2010.
- [6] M. Gitterman. The noisy oscillator: the first hundred years, from Einstein until now. World Scientific, 2005.
- [7] E. Clouet. Elastic energy of a straight dislocation and contribution from core tractions. *Philos. Mag.*, 89(19):1565–1584, 2009.
- [8] E. Clouet, L. Ventelon, and F. Willaime. Dislocation core energies and core fields from first principles. *Phys. Rev. Lett.*, 102:055502, 2009.
- [9] E. Clouet. Dislocation core field. I. modeling in anisotropic linear elasticity theory. *Phys. Rev. B*, 84(22):224111, 2011.
- [10] E. Clouet. Babel. http://emmanuel.clouet.free.fr/Programs/Babel/, 2010-2016.
- [11] P.-A. Geslin, R. Gatti, B. Devincre, and D. Rodney. Implementation of the nudged elastic band method in a dislocation dynamics formalism: application to dislocation nucleation. J. Mech. Phys. Solids, 108:49–67, 2017.
- [12] E. Bitzek. Thesis: Atomistic simulation of dislocation motion and interaction with crack tips and voids, 2006.