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# Elastic interaction between defects in thin and 2D films

P. Peyla[1] and C. Misbah[2,a]

[1] Laboratoire de Physique et de Modélisation des Milieux Condensés, Université Joseph Fourier (CNRS), BP 166, 38042 Grenoble Cedex 9, France
[2] GREPHE, Groupe de Recherche sur les Phénomènes Hors Équilibre, LSP, Université Joseph Fourier (CNRS), Grenoble I, Saint-Martin d'Hères, 38402 Cedex, France

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**Abstract.** Elastic interactions between defects is investigated at the surface of thin layers, a question on which we have given a brief account [P. Peyla *et al.* Phys. Rev. Lett. **82**, 787 (1999)]. Two isotropic defects do not interact in an unlimited medium, regardless of the spatial dimension, a result which can be shown on the basis of the Gauss theorem in electrostatics. Within isotropic elasticity theory, defects interact only (i) if they are, for example, at a surface (or at least if they feel a boundary), or if their action on the material is anisotropic (*e.g.* they create a non central force distribution, though the material elasticity is isotropic). It is known that two identical isotropic defects on the surface of a semi-infinite material repel each other. The repulsion law behaves as $1/r^3$($r$ = defects separation). We first revisit the Lau-Kohn theory and extend it to anisotropic defects. Anisotropy is found to lead to attraction. We show that in thin films defects may either attract or repel each other depending on the local geometric force distribution caused by the defect. It is shown that the force distribution (or more precisely the forces configuration symmetry) fixes the exponent in the power law $1/r^n$ (*e.g.* for a four-fold symmetry $n = 4$). We discuss the implication of this behaviour in various situations. We treat the interactions in terms of the symmetries associated with the defect. We argue that if the defects are isotropic, then their effective interaction in an unlimited 2D (or a thin film) medium arises from the induced interaction, which behaves as $1/r^4$ for any defect symmetry. We shall also comment on the contribution to the interaction which arises from flexion of thin films.

**PACS.** 68.35.Gy Mechanical properties; surface strains – 68.55.-a Thin film structure and morphology

## 1 Introduction

Elasticity, though it is by definition associated with *small* displacements of atoms around their equilibrium positions, it can drastically affect the macroscopic and mesoscopic behaviours of materials. For example, it is well known that a dislocation-free thin film which is epitaxially grown on a substrate may, after an initial layer by layer growth, break up into small islands, usually called *quantum dots*. This is the Stranski-Krastanov growth mode. A typical example is encountered during MBE growth of Ge/Si where the Ge film breaks into mounds after two to three mono-layers [1]. Other examples are known in the literature, and especially InGaAs-based materials. These systems are of much current technological importance [2]. The break-up of a layer by layer growth into mounds is mainly attributed to the *elastic relaxation*: due to the film/substrate lattice mismatch the film stores an elastic energy that is partially released by the formation of mounds. The stress-induced morphological instability has been recently the subject of several investigations (for a review see [3]). Besides energy, kinetics may play also a decisive role. It is important thus to know how a mobile atom on the surface (adatom) may feel the strain caused by pre-existing islands, steps, etc..., an interaction which should dictate the direction of motion for clustering. This means that the knowledge of elementary interactions is essential. This task also constitutes the first step for the determination of interactions of more extended defects, such as steps, islands, etc... We shall often refer to adatoms, inclusions, steps... as *defects*.

The study of the defect-defect interaction in the bulk is an old problem [4,5] which has given rise to a myriad of studies. The study of the interactions between surface defects (adatoms, steps...) is more recent [6,7]. It has been shown that two identical adatoms on a semi infinite solid repel each other according to the law $1/r^3$, where $r$ is the distance between the two adatoms. From this law it follows (see later) that two steps repel each other according to the law $1/\ell^2$, where $\ell$ is the inter-step distance, or that

[a] e-mail: chaouqi.misbah@ujf-grenoble.fr

an island of atoms $B$ which is in epitaxy on a substrate $A$ stores an elastic energy which is [8] $R\ln(R)$, where $R$ is the island radius, and so on. For the case of an island with a finite height, see [9].

There are several situations where one has to deal with thin films of a few atomic thicknesses, or with purely two dimensional objects. To cite but a few examples, many quantum wells are made of thin layers embedded in a matrix. If the film is soft in comparison to the underlying substrate the interaction between two defects is mainly mediated by the film. If the defect-defect separation is large in comparison to the film thickness the problem is effectively two dimensional. The same scenario occurs during growth of a relatively soft layer where adatom-adatom interaction on top of the soft layer is effectively of 2D nature. During Van der Waals epitaxy growth [10], the layered structure presents weak interaction at the heterojunction with the substrate, thus the deposited film behaves as a pure 2D medium. By now the fabrication of purely 2D solids is quite common and is of much current technological and fundamental importance. For example, carbon nanotubes and sheets [11] are purely two dimensional objects. The study of defect-defect interaction must be based on two dimensional elasticity. Similarly, 2D Langmuir monolayers [12] are two dimensional solids where the present study should be of interest. Finally, inclusions in biological membranes, like proteins, interact through the phospholipidic bilayer. There are fluid-like membranes where the interaction between inclusions is mediated by the membrane undulation [13], and elastic-like membranes (like in red blood cells for example – note in passing that here one usually needs to consider a nonlinear elastic law [14] for the membrane deformation) where the in-plane elastic deformation is decisive. In biology, it is well documented that biological cells are affected by the deformation of the substrate. For example, when fibroblasts are cultured on silicone rubber or collagen, they deform their substrate. If muscle cells are added to such a substrate, the cells become aligned [15]. For all these reasons a theory of defect-defect interaction in 2D seems necessary. A brief account on this topic has been given in [16].

As there is sparse information on several questions, we have felt it worthwhile at some places to give a comprehensive review on the problem of defects interactions. We shall first review the problem of defects interactions on a surface of semi-infinite medium. We extend the results of Lau and Kohn [6] to the case of anisotropic defects. We shall start with a qualitative discussion based of dimensional considerations. We then turn to the 2D problem. We shall show that two isotropic defects in an extended 2D medium have no interaction to leading order. The only possible interactions for isotropic defects in this case are (i) those arising because of the existence of a boundary, a situation encountered if the film extent is finite (defect images), (ii) the induced interaction, very much like the interaction between a neutral atom and an ion where the interaction is non-vanishing only because the ion induces a dipole on the neutral atom [17]. In the present case this means that the elastic modulus (or the force distribution of a defect) depends on the strain of the other defect. In that case it will be shown that the interaction behaves always like $1/r^4$, and it will be called *induced* or *nonlinear* interaction.

In reality, despite the fact that it can be assumed that a solid obeys isotropic elasticity (for example a hexagonal 2D structure does so), the defect has its own symmetry, that can be two-fold, three-fold, etc... We shall show that because of the low symmetry of the defect, two defects inserted in a 2D isotropic medium will interact with each other with a law which depends on the defect symmetry. For example, two defects having a two-fold axis of symmetry interact with a law behaving as $1/r^2$. For a three-fold symmetry they interact according to a law $1/r^3$, unless they are oriented in the same direction (the position of one of them can be obtained just by a pure translation of the other), in which case the interaction law behaves as $1/r^4$. For any other higher symmetry we find the following interaction $\sim 1/r^n$, with $n > 4$. In that case one should take the induced interaction, which is of longer range ($1/r^4$), into consideration. This will be shown briefly. Finally since thin films may undergo out-of plane deformations, the interaction *via* the film undulation (flexion) becomes a possible source of interaction. We shall present a discussion on this effect.

The scheme of this paper is as follows. In Section 2 we give a simple argument in order to evaluate the defect-defect interaction on a surface of a semi-infinite solid. In Section 3 we give the general way of evaluating the interaction energy, and in Section 4 we illustrate the general method for a semi-infinite medium. We revisit the classical theory by allowing for a non central force distribution. Section 5 is dedicated to the special situation where isotropic defects are present within an unlimited medium, and it is shown that the linear interaction vanishes to all order in the multi-polar expansion. Section 6 focuses on 2D and thin films. A conclusion, and a discussion on the induced interaction as well as on the effect of interaction mediated by flexion is given in Section 7. The Appendix contains a general way for computing the elastic interaction based on the use of the Green's function along with symmetries associated with the defect.

## 2 Dimensional considerations

In this section we present simple physical arguments and dimensional considerations in order to derive the defect-defect interaction on the surface of a 3D solid. Precise and quantitative expressions are derived in the next sections. Let us consider the situation where a localized defect (atom or molecule) is present on the surface of an elastic medium (a semi-infinite solid). The solid atoms exert on the adatom a set of forces $\{\mathbf{f}^{(n)}\}$ (coming from nearest neighbors etc..., and $n$ denotes the forces number $n$ among a total number $N$) (Fig. 1). Since the defect is at equilibrium and it is considered as a point defect, mechanical equilibrium requires the total force acting on it be zero: $\mathbf{f}_T = \sum_{n=1}^{N} \mathbf{f}^{(n)} = 0$. Due to the fact that we

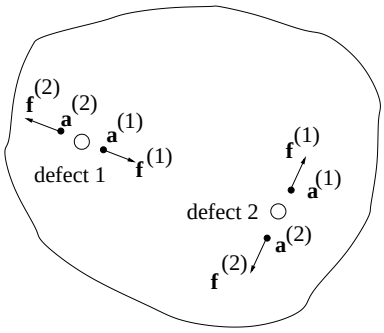


**Fig. 1.** Defects (open circles) exerting forces on their nearest neighbors (filled circles). The medium between the defects is considered as a continuous elastic body.

consider defects with a center of symmetry (but not necessarily spherical symmetry), the mechanical torque must vanish as well, $\Gamma = \sum_{n=1}^{N} \mathbf{r}^{(n)} \times \mathbf{f}^{(n)} = 0$. Note that our reasoning can refer either to the forces created by the defect on the substrate, or to those due to the substrate on the defect; this does not matter since due to the action and reaction principle the total force is zero.

If the response of the solid to a given force is known, then that due to a force distribution can straightforwardly be derived, owing to the superposition principle in elasticity theory. A force creates a displacement in the solid which obeys the Lamé equation (see next sections). From a dimensional point of view the Lamé equation is equivalent to the Poisson one encountered in electrostatics. We have the equivalence between the displacement and the potential and between the force and the charge. That is, dimensionally, the Lamé equation reads

$$\nabla^2 \mathbf{u} \sim \mathbf{f} \cdot \delta(\mathbf{r}), \tag{1}$$

where $\mathbf{f} \cdot \delta(\mathbf{r})$ is a localized force, equivalent to a point charge, and $\mathbf{u}$ is the displacement created by this force. As we know from electrostatics in 3D

$$\mathbf{u} \sim \mathbf{f}/r. \tag{2}$$

For definiteness let us consider a very simple example (Fig. 2). We suppose that the crystal reacts with a set of two forces $\mathbf{f}^{(1)}\delta(x-a)$ and $\mathbf{f}^{(2)}\delta(x+a)$ (a force dipole) directed along the surface in the $Ox$ direction. Equilibrium imposes $\mathbf{f}^{(1)} = -\mathbf{f}^{(2)} = \mathbf{f}$. Due to the linearity of the Lamé equation, this dipole creates a total displacement field $\mathbf{u}_T(x)$ which is a linear superposition of the displacements $\mathbf{u}$ created at a distance $x$ by each force, $\mathbf{f}^{(1)}$ and $\mathbf{f}^{(2)}$. As every vector is parallel to the $x$-axis, we drop the vector notation. We have

$$u_T(x) = u(x-a) + u(x+a) \sim \frac{f}{x-a} - \frac{f}{x+a}. \tag{3}$$

Assuming that $a \ll x$, we can write to leading order:

$$u_T(x) \sim (2af)\frac{\partial u}{\partial x} \sim \frac{2af}{x^2}. \tag{4}$$

Note that the sign depends on the force orientation and we shall first omit this in this qualitative argument. In order


**Fig. 2.** Force dipole.

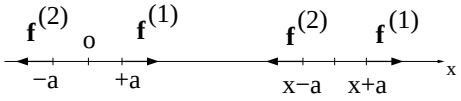


**Fig. 3.** Force dipole. Two parallel dipoles along the $x$-axis.

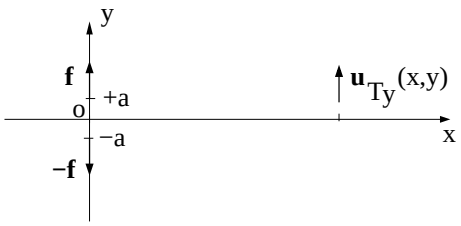


**Fig. 4.** Force dipole. Total displacement created by a dipole parallel to the $y$-axis.

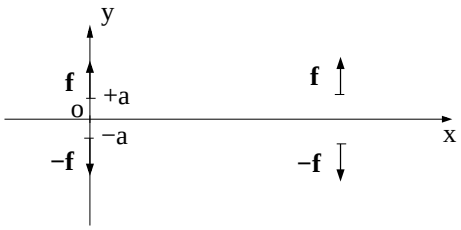


**Fig. 5.** Force dipole. Two dipoles parallel to $y$-axis located on the $x$-axis.

to prepare the general discussion in the next section, we find it convenient to introduce the analogue of a dipolar momentum $\Omega$ (which is a force times the position vector). Here, in this simple geometry we introduce the quantity $\Omega = f^{(1)}a - f^{(2)}a = 2af$ (see next paragraph for the general definition of $\Omega$ which becomes a tensor). Equation (4) becomes:

$$u_T \sim \Omega/x^2. \tag{5}$$

The interaction energy is proportional to the force multiplied by the displacement. We must multiply the displacement due to the first atom by the forces of the second atom so that only the interaction is counted (and not the self energy). If a second identical atom is present at a distance $x$ from the first one (Fig. 3), the interaction energy is thus:

$$F_{int} \sim (fu_T(x+a) - fu_T(x-a)) \sim 4f^2a^2\frac{\partial^2 u}{\partial x^2}, \tag{6}$$

leading to

$$F_{int} \sim \Omega^2/x^3. \tag{7}$$

This is a classical result (Lau and Kohn [6]).

Consider now the effect of vertical forces (Fig. 6) on a semi-infinite elastic solid (the solid is in the domain $z < 0$, and the surface is located at $z = 0$, Fig. 6). For the torque to vanish a set of three forces at least is necessary (Fig. 6).

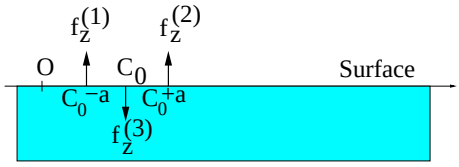


**Fig. 6.** Surface defect applying vertical forces (*i.e.* perpendicular to the surface). Forces are applied at surface.

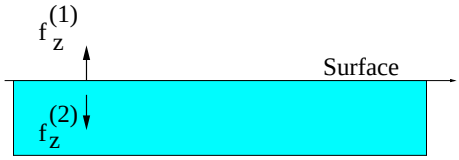


**Fig. 7.** Like in Figure 2 but forces are applied at and below the surface.

We must have $\Gamma_x = 0$, $\Gamma_y = (-a+c_0)f_z^{(2)} + (c_0+a)f_z^{(1)} + c_0 f_z^{(3)} = 0$ ($c_0$ is an arbitrary origin) and $\Gamma_z = 0$. The other mechanical constraint is $f_z = f_z^{(1)} + f_z^{(2)} + f_z^{(3)} = 0$. The vanishing of $\Gamma$ is independent of the origin $c_0$. Here, the dipolar momentum $\Omega = f(-a) + (-2f)0 + fa = 0$. This is in fact a quadrupole, and therefore the vertical forces applied at the surface contributes to higher order terms, in comparison to the parallel forces, in the dipolar expansion, as explained above. Following the same lines as above, we obtain the total displacement $u_{Tz}(x)$ created by the first defect:

$$u_{Tz} = u_z(x+a) + u_z(x-a) - 2u_z(x) = a^2 \frac{\partial^2 u_z(x)}{\partial x^2},$$

where $u_z(x)$ is the displacement created by a force $f_z = f$ localized at the surface of a semi-infinite solid. As before the interaction energy is:

$$\begin{aligned} F_{int} &\sim -f\left[u_{Tz}(x-a) + u_{Tz}(x+a) - 2u_{Tz}(x)\right] \\ &\sim -fa^2 \frac{\partial^2 u_{Tz}(x)}{\partial x^2} \\ &\sim -fa^4 \frac{\partial^4 u_z}{\partial x^4}. \end{aligned} \tag{8}$$

$u_z(x)$ is given by the result obtained from dimensional considerations considered above, ($u_z(x) \sim f/x$ in 3D), the interaction is thus

$$F_{int} \sim f^2 a^4 \frac{1}{x^5}.$$

As anticipated above, this is negligible in comparison with the in-plane forces interaction (7). However, if at least one of the vertical forces is applied under the surface (Fig. 7), then two forces are sufficient in order to fulfill the demand of a vanishing torque $\Gamma$. In that case, Kern and Krohn [18] have shown that the lowest order term of the dipolar expansion is still $F_{int} \sim \Omega^2/x^3$. This result can also be derived along the same lines presented above.

The geometry of the forces associated with a point defect is dictated by the symmetry of the underlying crystal *i.e.* by the chemical bonds geometry, and by the symmetry of the defect itself. If one considers an isotropic medium, then what matters is the defect symmetry. In this paper we shall mainly address the basic physical ideas rather than to treat a long list of specific examples.

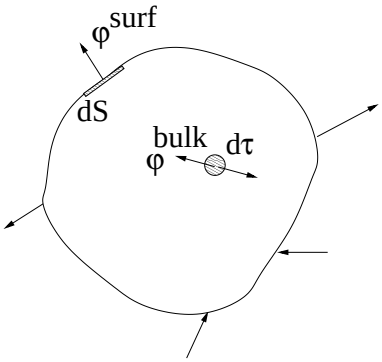


**Fig. 8.** A schematic view of surface and bulk forces $\varphi$ applied to an elastic body. A surface element is d$S$ and a volume element is d$\tau$.

## 3 Elastic free energy

In this section we give the precise free energy $F$ of an elastic body as a function of the displacements and the applied forces acting on the body. This expression is useful in what follows. Despite the fact that the derivation given below is based on general considerations which are rather classical in elasticity theory, we have felt it worthwhile to devote a short paragraph to this question and keep the paper both concise and self-contained.

We consider a finite elastic body of volume $V$ enclosed by a surface $S$. The applied forces (Fig. 8) can be split into surface forces (forces per unit surface): $\boldsymbol{\varphi}^{surf}$ acting on a surface element d$S$ of the body (contact forces, surface defects, adatoms, ...) and bulk forces (forces per unit volume): $\boldsymbol{\varphi}^{bulk}$ acting on a volume element d$\tau$ of the body (gravity, bulk defects, dislocations, impurities, ...). Let us denote by $\sigma_{ij}$ the stress tensor and by

$$\varepsilon_{ij} = \left(\partial u_i/\partial x_j + \partial u_j/\partial x_i\right)/2 \tag{9}$$

the strain tensor, where $u_i$ is the $i$th component of the displacement. The two tensors $\sigma_{ij}$ and $\varepsilon_{ij}$ are linearly related by Hooke's law. The total free energy $F$ can thus be expressed as follows [19]:

$$F = \frac{1}{2}\int_V \sigma_{ij}\varepsilon_{ij}\,\mathrm{d}\tau - \int_V \varphi_i^{bulk}\,u_i\,\mathrm{d}\tau - \oint_S \varphi_i^{surf}\,u_i\,\mathrm{d}S. \tag{10}$$

The first term is the energy associated with the solid distortion, while the two other terms account for the mechanical work due to the forces associated, for example, with defects. Note that repeated subscripts are to be summed over. Using the definition of $\varepsilon_{ij}$ we can write

$$\frac{1}{2}\int_V \sigma_{ij}\varepsilon_{ij}\,\mathrm{d}\tau = \frac{1}{2}\oint_S \sigma_{ij}\,u_i\,\mathrm{d}S_j - \frac{1}{2}\int_V \frac{\partial \sigma_{ij}}{\partial x_j} u_i \mathrm{d}\tau. \tag{11}$$

Here we have integrated by parts and used the divergence theorem.

Upon substitution into equation (10), we obtain:

$$F = \frac{1}{2}\oint_S \sigma_{ij}\, u_i \,\mathrm{d}S_j - \frac{1}{2}\int_V \frac{\partial \sigma_{ij}}{\partial x_j} u_i \mathrm{d}\tau - \int_V \varphi_i^{int}\, u_i \,\mathrm{d}\tau - \oint_S \varphi_i^{surf}\, u_i \,\mathrm{d}S. \quad (12)$$

Mechanical equilibrium requires:

$$\begin{cases} \dfrac{\partial \sigma_{ij}}{\partial x_j} + \varphi_i^{bulk} = 0 \\ \sigma_{ij}\mathrm{d}S_j = \varphi_i^{surf}\mathrm{d}S. \end{cases} \quad (13)$$

The first equation is nothing but the bulk equilibrium elastic equation [19], while the second one refers to the boundary condition at the surface.

With the help of the above equilibrium equations, equation (12) assumes the following final form:

$$F = -\frac{1}{2}\int_V \varphi_i^{bulk}\, u_i \,\mathrm{d}\tau - \frac{1}{2}\oint_S \varphi_i^{surf}\, u_i \,\mathrm{d}S. \quad (14)$$

Note that in the derivation of the interaction energy we must subtract the self energy. That is to say, we must subtract from the above expression the energy due to singles defects, as will be written below.

### 3.1 Interaction energy

We consider a set of defects each being represented by a set of localized forces ($\delta$-functions) $\mathbf{f}^{(n)}$ applied at different positions $\mathbf{a}^{(n)}$. Expression (14) becomes then:

$$F = -\frac{1}{2}\sum_n \mathbf{f}^{(n)}\mathbf{u}^{(n)}. \quad (15)$$

The sum $n$ runs over each force associated with each defect. Note that the distinction between surface forces and volume forces is not necessary, since it is sufficient to write the forces as $\delta$-functions either at the surface or in the bulk. In order to use the above expression, we only need to evaluate the displacement field $\mathbf{u}^{(n)}$ created by a localized force $\mathbf{f}^{(n)}$. Very much like in electrostatics, the knowledge of the potentials created by individual charges is sufficient for the determination of the energy. This type of interaction will be referred to as a *linear interaction*. Note that we have not yet substrated the self energy.

The above expression is used in order to calculate the interaction energy of two defects represented by the sets of localized forces $\{f^{(n)}\}$ and $\{f^{(m)}\}$ (Fig. 9), where the superscripts $n$ and $m$ refer to the $n$th force due to the first defect and the $m$th one due to the second defect, respectively. Let $\mathbf{u}_{T1}(\mathbf{r})$ denote the total displacement created by the first defect, and $\mathbf{u}_{T2}(\mathbf{r})$ the one created by the second defect:

$$\mathbf{u}_{T\alpha}(\mathbf{r}) = \sum_{n\in defect\,\alpha} \mathbf{u}^{(n)}(\mathbf{r}).$$

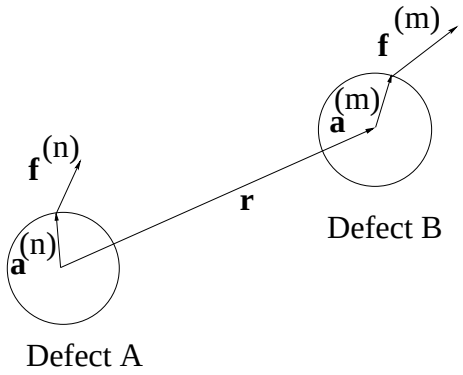


**Fig. 9.** Two defects $A$ and $B$. Superscripts $n$ and $m$ are devoted to $A$ and $B$ respectively (see text).

By using equation (15), we can write the total elastic energy as:

$$F = F_{self} + F_{int}.$$

$F_{self}$ is the sum of the self energy of each defect:

$$F_{self} = -\frac{1}{2}\sum_n \mathbf{f}^{(n)} \cdot \mathbf{u}_{T1}\left[\mathbf{a}^{(n)}\right] - \frac{1}{2}\sum_m \mathbf{f}^{(m)} \cdot \mathbf{u}_{T2}\left[\mathbf{a}^{(m)}\right].$$

We have written explicitly the argument of the displacement field in order to avoid confusion: $[a^{(n)}]$ means that the displacement is evaluated at a distance equal to $a^{(n)}$, and this distance is counted from the defect center of forces (Fig. 5). $F_{int}$ is the interaction energy:

$$F_{int} = -\frac{1}{2}\sum_n \mathbf{f}^{(n)} \cdot \mathbf{u}_{T2}\left[\mathbf{a}^{(n)} - \mathbf{r}\right] - \frac{1}{2}\sum_m \mathbf{f}^{(m)} \cdot \mathbf{u}_{T1}\left[\mathbf{a}^{(m)} + \mathbf{r}\right]. \quad (16)$$

In equation (6) we have a simple example that helps to understand the arguments entering the elastic field. Then the task will be to expand the displacement field for $a/r$ being small (multi-polar expansion).

This expression will be used throughout this paper, the question being now to express the displacement field created by a localized force applied to an elastic body of a given geometry. In this paper we shall consider essentially three cases, (i) an infinite 3D body, (ii) a semi-infinite solid, and (iii) a 2D infinite body or thin layer.

## 4 Revisited theory for a semi-infinite solid

In this paragraph we revisit the problem of defects interactions for semi-infinite solid. We extend the classical Lau-Kohn [6] theory to anisotropic defects. Unlike electrostatics, the dipolar moment is a tensor of which each

component is defined as:

$$\Omega_{\alpha\beta} = \sum_{n=1}^{N} f_\alpha^{(n)} a_\beta^{(n)}. \tag{17}$$

The quantity $(f_x^{(n)}, f_y^{(n)}, f_z^{(n)})$ designates the set of $N$ forces ($n = 1...N$) located at $(a_x^{(n)}, a_y^{(n)}, a_z^{(n)})$, $(\alpha, \beta) = (x, y, z)$. We can check that equation (17) is coherent with the one introduced in the above paragraph for the special case of a dipole of forces with $n = 2$, $a_x^{(1)} = -a$, $a_x^{(2)} = +a$, $a_y^{(1)} = a_y^{(2)} = a_z^{(1)} = a_z^{(2)} = 0$, $f_x^{(1)} = -f$ and $f_x^{(2)} = +f$, leading to $\Omega_{xx} = (-f)(-a) + fa = 2fa$, the other components of the tensor $\Omega$ being identically zero.

In 3D, the Lamé equation for the displacement $\mathbf{u}$ reads [19]

$$\nabla^2 \mathbf{u} + \frac{1}{1-2\sigma} \nabla(\nabla \mathbf{u}) = -\frac{2(1+\sigma)}{E} \mathbf{f}\delta(\mathbf{r}), \tag{18}$$

where $\sigma$ is Poisson's coefficient (dimensionless) and $E$ the Young modulus (having the dimension of a force per unit surface), $\mathbf{f}\delta(\mathbf{r})$ is a force per unit volume localized at the origin, and $\mathbf{r}(x, y, 0)$ is the position vector on the surface. For a semi-infinite solid the expression of $\mathbf{u}(\mathbf{r})$ evaluated at the surface takes the following form [19]:

$$\begin{cases} u_x(x,y,0) = \dfrac{1+\sigma}{2\pi E}\dfrac{1}{r}\left[\dfrac{(2\sigma-1)x}{r} f_z + 2(1-\sigma) f_x \right. \\ \qquad\qquad \left. + \dfrac{2\sigma x}{r^2}(x f_x + y f_y)\right] \\ u_y(x,y,0) = \dfrac{1+\sigma}{2\pi E}\dfrac{1}{r}\left[\dfrac{(2\sigma-1)y}{r} f_z + 2(1-\sigma) f_y \right. \\ \qquad\qquad \left. + \dfrac{2\sigma y}{r^2}(x f_x + y f_y)\right] \\ u_z(x,y,0) = \dfrac{1+\sigma}{2\pi E}\dfrac{1}{r}\left[2(1-\sigma) f_z \right. \\ \qquad\qquad \left. + (1-2\sigma)\dfrac{1}{r}(x f_x + y f_y)\right]. \end{cases} \tag{19}$$

As seen before, a defect is associated with a set of forces $\mathbf{f}^{(n)} = (f_x^{(n)}, f_y^{(n)}, f_z^{(n)})$ applied at the surface at positions $\mathbf{a}^{(n)}$ within an area of typical size $a$. We shall denote the total displacement due to a defect by $\mathbf{u}_T(x, y, 0)$. Considering that the total force $\mathbf{f} = \sum_n \mathbf{f}^{(n)}$is zero, we find that $\mathbf{u}_T$ at a distance $r \gg a$ is given, to first order in $\Omega_{ij}$, by:

$$\begin{cases} u_{Tx}(x,y,0) = \dfrac{1+\sigma}{2\pi E}\dfrac{1}{r^2}\left[(2\sigma-1)\left(-\Omega_{zx} \right.\right. \\ \qquad \left.\left. + 2\dfrac{x^2\Omega_{zx} + xy\Omega_{zy}}{r^2}\right) \right. \\ \qquad + 2(1-\sigma)\dfrac{x\Omega_{xx} + y\Omega_{xy}}{r} \\ \qquad - 2\sigma\,\dfrac{2x\Omega_{xx} + y\Omega_{yx} + x\Omega_{yy}}{r} \\ \qquad \left. + 6\sigma\dfrac{x^3\Omega_{xx} + yx^2\Omega_{xy} + x^2y\Omega_{yx} + xy^2\Omega_{yy}}{r^3}\right] \\ u_{Ty}(x,y,0) = \dfrac{1+\sigma}{2\pi E}\dfrac{1}{r^2}\left[(2\sigma-1)\left(-\Omega_{zy} \right.\right. \\ \qquad \left.\left. + 2\dfrac{y^2\Omega_{zy} + yx\Omega_{zx}}{r^2}\right) \right. \\ \qquad + 2(1-\sigma)\dfrac{y\Omega_{yy} + x\Omega_{yx}}{r} \\ \qquad - 2\sigma\,\dfrac{2y\Omega_{yy} + x\Omega_{xy} + y\Omega_{xx}}{r} \\ \qquad \left. + 6\sigma\dfrac{y^3\Omega_{yy} + xy^2\Omega_{yx} + y^2x\Omega_{xy} + yx^2\Omega_{xx}}{r^3}\right] \\ u_{Tz}(x,y,0) = \dfrac{1+\sigma}{2\pi E}\dfrac{1}{r^2}\left[(1-2\sigma)\left(-\Omega_{xx} - \Omega_{yy} \right.\right. \\ \qquad \left.\left. + 2\dfrac{x^2\Omega_{xx} + xy\,(\Omega_{xy} + \Omega_{yx}) + y^2\Omega_{yy}}{r^2}\right) \right. \\ \qquad \left. + 2(1-\sigma)\dfrac{x\Omega_{zx} + y\Omega_{zy}}{r}\right]. \end{cases} \tag{20}$$

Now, let us apply the above expression (20) to some simple cases and derive the exact expression of the interaction energy.

i) Consider a force dipole which is parallel to the $x$-axis (Fig. 2). Here only $\Omega_{xx} = 2\,f\,a$ enters. We get for the total displacement:

$$u_{Tx}(x,0,0) = \frac{1+\sigma}{\pi E x^2}\Omega_{xx} = 2\frac{1+\sigma}{\pi E x^2} f\,a, \tag{21}$$

from which it is easy to evaluate the interaction energy between two dipoles which are parallel to the $x$-axis (see Fig. 3) by using equation (16):

$$\begin{aligned} F_{int} = -\frac{1}{2}[&f\,u_{Tx}(x+a,0,0) - f\,u_{Tx}(x-a,0,0) \\ &+ f\,u_{Tx}(-x+a,0,0) - f\,u_{Tx}(-x-a,0,0)]. \end{aligned} \tag{22}$$

Note that here we have $u_{Tx}(x+a,0,0) = u_{Tx}(-x-a,0,0)$ and $u_{Tx}(x-a,0,0) = u_{Tx}(-x+a,0,0)$. Considering that the two dipoles are far apart from each other (*i.e.* $x \gg a$), expansion of (22) to leading order in $a$, yields:

$$F_{int} = 8\frac{1+\sigma}{\pi E}\frac{a^2 f^2}{x^3}, \tag{23}$$

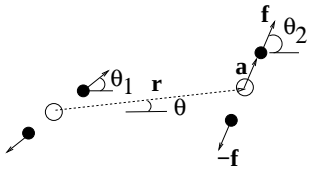


**Fig. 10.** Two dipoles of force in the plane of the film, general situation.

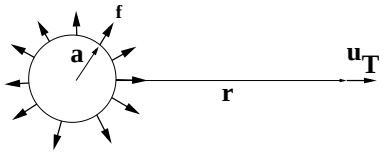


**Fig. 11.** An isotropic defect (a sphere in 3D and a disk in 2D). Total displacement created by an isotropic defect.

which is a repulsive interaction.

ii) Now, consider a force dipole which is parallel to the $y$-axis (Fig. 4). Here only $\Omega_{yy} = 2\,f\,a$ enters in the calculation. We get for the total displacement:

$$u_{Ty}(x,y,0) = \frac{1+\sigma}{\pi E r^5}\Omega_{yy}\left[y^3 + (1-3\sigma)x^2 y\right] = 2\frac{1+\sigma}{\pi E r^5} f\,a\left[y^3 + (1-3\sigma)x^2 y\right]. \quad (24)$$

Once again, we evaluate the interaction energy between two dipoles which are parallel to the $y$-axis (see Fig. 5) by using equation (16):

$$F_{int} = -\frac{1}{2}[f\,u_{Ty}(x,a,0) - f\,u_{Ty}(x,-a,0) + f\,u_{Ty}(-x,a,0) - f\,u_{Ty}(-x,-a,0)]. \quad (25)$$

For a large separation between the two defects (*i.e.* $x \gg a$), we obtain from (25) to leading order in $a$:

$$F_{int} = -4\frac{(1+\sigma)(1-3\sigma)}{\pi E}\frac{a^2 f^2}{r^3}\cdot \quad (26)$$

If $\sigma < 1/3$ (the usual range for $\sigma$ lies within $0.25 < \sigma < 0.3$) the interaction is attractive, and it is repulsive otherwise.

iii) Consider a generalization of the two above studied cases i) and ii) where two force dipoles make angles $\theta_1$ and $\theta_2$ with the vector joining them (Fig. 10). Here, the non-vanishing components of the dipolar tensor are:

$$\begin{cases} \Omega_{xx} = 2\,f\,a\,\cos^2\theta_1 \\ \Omega_{yy} = 2\,f\,a\,\sin^2\theta_1 \\ \Omega_{xy} = \Omega_{yx} = 2\,f\,a\,\cos\theta_1\,\sin\theta_1 \end{cases}$$

and a similar expression for the second dipole with the substitution $\theta_1 \to \theta_2$. Following the same procedure we get:

$$\begin{cases} u_{Tx} = \dfrac{a\,f\,(1+\sigma)}{\pi E r^5}\left[(1-\sigma)\,x r^2 + (1+\sigma)\,x^3\cos 2\theta_1 + (1-5\sigma)\,xy^2\cos 2\theta_1 + y(r^2 + 4\sigma x^2 - 2\sigma y^2)\,\sin 2\theta_1\right] \\ u_{Ty} = \dfrac{a\,f\,(1+\sigma)}{\pi E r^5}\left[(1-\sigma)\,y r^2 - (1+\sigma)\,y^3\cos 2\theta_1 - (1-5\sigma)\,x^2 y\cos 2\theta_1 + y(r^2 + 4\sigma x^2 - 2\sigma y^2)\,\sin 2\theta_1\right]. \end{cases} \quad (27)$$

It is a simple matter to see that the special cases treated above are recovered. From equation (16), some algebraic manipulations allow us to write the energy as

$$F_{int} = \frac{1+\sigma}{2\pi E}\frac{a^2 f^2}{r^3}\Im(\theta_1,\theta_2), \quad (28)$$

with

$$\Im(\theta_1,\theta_2) = 2(1-\sigma) + 6(1-\sigma)(\cos 2\theta_1 + \cos 2\theta_2) + (2-\sigma)\cos 2(\theta_1-\theta_2) + 15\sigma\cos 2(\theta_1+\theta_2). \quad (29)$$

Expression (28) reduces to (23) or (26) for $\theta_1 = \theta_2 = 0$ or $\theta_1 = \theta_2 = \frac{\pi}{2}$ respectively.

It must be emphasized that the interaction energy may either be attractive or repulsive depending on the values of $\theta_1$ and $\theta_2$. This markedly contrasts with the classical law derived by Lau and Kohn [6] where the interaction is only repulsive. This is traced back to the fact that the defects considered there are assumed to be isotropic (see below).

iv) Let us finally treat the case of an isotropic defect (Fig. 11). The only non-vanishing components of the dipolar momentum are

$$\begin{cases} \Omega_{xx} = \int f_x\,x\mathrm{d}\theta = \int f\,a\,\cos^2(\theta)\,\mathrm{d}\theta = \pi f a \\ \Omega_{yy} = \int f_y\,y\mathrm{d}\theta = \int f\,a\,\sin^2(\theta)\,\mathrm{d}\theta = \pi f a. \end{cases} \quad (30)$$

Plugging this into equation (20), we arrive at

$$u_{Tx}(x,0,0) = \frac{(1-\sigma^2)}{\pi E x^2}\Omega_{xx} = \frac{(1-\sigma^2)}{E x^2} f\,a$$

and similar (isotropic) expressions for the other components. Here we consider the field at a point lying on the axis $ox$. Since the defect is isotropic the field is invariant under a rotation around the defect. Thus, the full displacement vector is given by:

$$\mathbf{u}_T(\mathbf{r}) = \frac{(1-\sigma^2)}{E r^3} f\,a\,\mathbf{r}, \quad (31)$$

where $\mathbf{u}_T$ is the displacement vector parallel to the surface and is created by an isotropic defect at a point $\mathbf{r} = (x,\,y,\,0)$ (Fig. 11). Note that, here, the $z$-component of the displacement is not needed since it does not contribute to the scalar product in (16). If another identical defect is located at a distance $r \gg a$, the interaction energy $F_{int}$ between the two defects (Fig. 12) is straightforwardly deduced by using the same procedure detailed

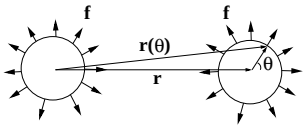


**Fig. 12.** The case of two isotropic defects.

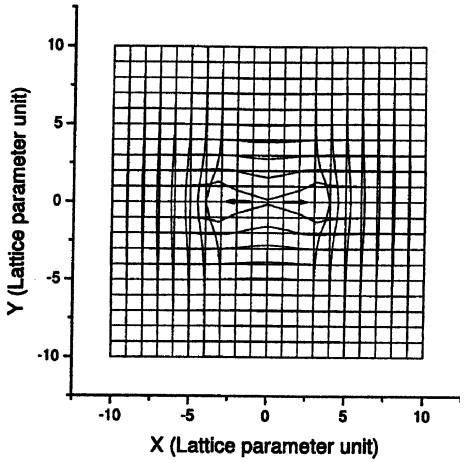


**Fig. 13.** Deformation of a square lattice by a force dipole parallel to the $x$-direction.

in i):

$$F_{int} = \frac{\pi(1-\sigma^2)}{Er^3} f^2 a^2. \tag{32}$$

This is the result of Lau and Kohn [6].

By comparing (28) and (32), we see that in the case of a dipole we can have both attractive (Eq. (26)) or repulsive (Eq. (23)) interactions, whereas for an isotropic defect the interaction is always repulsive (Eq. (32)). This result can be interpreted by considering the lattice deformation induced by a defect. In the case of a defect (A) which exerts a force dipole by pushing atoms around it, we can see in Figure 13 that far from the dipole the lattice feels a compression in the $x$-direction and a tension in the $y$-direction. Thus if a second (identical) defect (B) is located along the $x$-direction, it will enhance the compressive deformation between the two defects. As a consequence the presence of (B) is not favorable, and a repulsion results. Conversely, if (B) is located along the $y$-direction (*i.e.* on top of defect A in Fig. 13), it has a tendency to attenuate the tensile strain, and thus its presence in the vicinity of (A) may become favorable: (A) and (B) may attract each other along the $y$-direction. Now, if the defect exerts a set of four forces around it, we can see in Figure 14 that the lattice is roughly isotropically compressed everywhere and therefore, it is unfavorable for a second identical defect to approach the first one because whatever its position is, it would increase the compression. It is a simple exercise to show that the Lau and Kohn result is qualitatively valid for a four-fold symmetry (that is to say for any symmetry which is equal or higher than a four-fold one – or $C_4$ in the usual group theory notation) we recover, apart from a

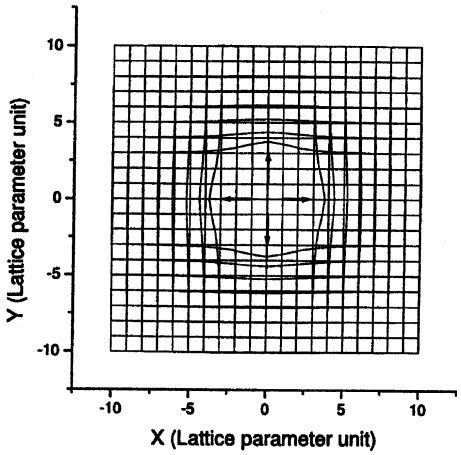


**Fig. 14.** Deformation of a square lattice by a four fold force distribution.

numerical factor, a similar result as for isotropic defects:

$$F_{int} = \frac{2f^2a^2(1-\sigma^2)}{\pi E r^3}. \tag{33}$$

## 5 The special case of isotropic defects in unbounded isotropic solids

If the solid is unbounded (that is, if we can ignore the presence of the surface), it is a simple matter to show that the interaction energy between two defects vanishes identically. In the case of a semi-infinite solid (infinite solid cut by a plane) the translational invariance is broken along the direction perpendicular to the surface, leading to some notable differences with the unbounded 3D solid. When a localized force $\mathbf{f}\delta(\mathbf{r})$ is applied in an infinite 3D elastic body, it creates a displacement $\mathbf{u}(\mathbf{r})$ given by [19]:

$$\mathbf{u} = \frac{(1+\sigma)}{8\pi E(1-\sigma)} \left[ \frac{(3-4\sigma)\mathbf{f} + \mathbf{n}(\mathbf{n}\cdot\mathbf{f})}{r} \right], \tag{34}$$

where $\mathbf{n}$ is a unit vector parallel to $\mathbf{r}$. Consider now an isotropic defect. The force distribution associated with it is given by $\mathbf{f} = f\delta(r-a)\mathbf{r}/r$. This defect enjoys the spherical symmetry in 3D (resp. a circular symmetry for a 2D solid as we shall be concerned with later). Expanding $\mathbf{u}$ to first order in $a$ and integrating on the surface of the sphere of radius $a$ around the defect, we get a total displacement:

$$\mathbf{u}_T = \frac{af(1+\sigma)(1-2\sigma)\mathbf{r}}{3E(1-\sigma)r^3}. \tag{35}$$

Because of the spherical symmetry of the defect, the total field is a divergence free so that the Lamé equation of the total field obeys $\Delta\mathbf{u_T} = \mathbf{0}$ [19]. As $\mathbf{u_T}$ is a solution of the Laplace equation that vanishes at infinity, and due to the uniqueness of the solution, $\mathbf{u_T}$ is the exact solution.

The interaction energy between this defect and another one located at distance $r$ is given by

$$F_{int} = -\oint_{\mathcal{C}} \mathbf{u}_T \cdot \mathbf{f}\, \mathrm{d}\Omega, \tag{36}$$

where the integration runs over $\mathcal{C}$, the closed surface of the second defect in 3D (resp. contour in 2D), and $d\Omega$ designates the solid angle. In view of the Gauss theorem (in 3D or in 2D, and actually in any dimension), this contribution vanishes identically! This is also easily checked since

$$\nabla \cdot \mathbf{u}_T = 0. \tag{37}$$

That is to say, two defects with isotropic forces distribution in an infinite and isotropic medium do not interact elastically [4]. Note that the semi-infinite case is quite different since, despite the fact that $\mathbf{u}_T$ is still given by $\sim 1/r^2$ (see Eq. (31)), $\mathcal{C}$ is no longer a closed surface but a closed contour which lies in the surface plane, implying that the Gauss theorem can not be used. As a consequence, isotropic defects at the surface of a semi-infinite solid do interact, as we have seen explicitly (Eq. (32)).

It might seem quite strange, even for an infinite solid, to admit that the presence of an isotropic defect would not feel another defect setting at some distance, since both of them will, beyond any doubt, distort the medium. This can be understood by noting that an isotropic defect in the solid changes the volume [20] (no shear strain) by an amount $\Delta V$, and that the interaction energy between the defects is proportional to $\Delta V$. For an infinite volume there is no volume change (in some sense the compression or dilatation produced locally is always compensated at infinity), and thus the interaction vanishes exactly, as shown above.

For a finite volume the problem must be solved with appropriate boundary conditions where defects can interact through their images [20]. The total elastic energy $F_T^{Finite}$ of two isotropic defects in a 3D finite medium of size $L$, can be written as:

$$F_T^{Finite} = 2F_{self}^{Finite} + F_{int}^{Finite} \tag{38}$$

where $F_{self}^{Finite}$ is the self-energy of a defect and $F_{int}^{Finite}$ the interaction energy. Assuming that the defect is a spherical hole of radius $a$, with a pressure $p$, near the center of an elastic sphere of radius $L$, it can be shown [19] that

$$F_{self}^{Finite} = F_{self}^{\infty} + A/L^3$$

where $A = 3p^2\pi(1-\sigma)a^6/E$ and $F_{self}^{\infty} = p^2\pi(1+\sigma)a^3/E$, $F_{self}^{\infty}$ is the self-energy of a defect in an infinite medium [4]. This finite system is equivalent to an infinite system, with the same two isotropic defects plus a certain number $\aleph$ of images. The total elastic energy is thus given by:

$$F_T^{\infty} = (2+\aleph)F_{self}^{\infty}. \tag{39}$$

There is no interaction term, because as mentioned above, in an infinite medium, defects do not interact. As $F_T^{\infty}$ (Eq. (39)) and $F_T^{Finite}$ (Eq. (38)) must be identical, we obtain:

$$F_{int}^{Finite} = -2A/L^3 + \aleph F_{self}^{\infty}. \tag{40}$$

For sufficiently large values of $L$, $F_{int}^{Finite} \to 0$, leading to $\aleph \to 2A/(F_{self}^{\infty}L^3)$. Therefore, when the size $L$ of the system is large in comparison with the distance between defects, $F_{int}^{Finite}$ gives a vanishingly small ($\sim 1/L^3$) contribution. An equivalent argument in two dimensions leads to an interaction which is typically of the order $\sim 1/L^2$. Thus, as far as the separation between the defects is small in comparison to their distance from the boundary, two isotropic defects have a vanishingly small interaction.

Hitherto, the interaction referred to concerns the so called *linear interaction*, in that it is additive (like in electrostatics). There is in reality a *non linear interaction* or the *induced one* on which we shall comment on in the section devoted to discussion. Let us for the moment continue with the linear interaction. According to the above discussion it is clear that when one considers a 2D solid (or thin enough films) or a 3D one, isotropic defects have no linear interactions, and one must ask the question – besides the induced interaction – whether there is a possible source of linear interaction. It will be seen here that this is the case when the defect has a low enough symmetry, like a dipole, tripole, quadrupole etc..., and it is only when the defect has a $\infty$-pole distribution that the interaction vanishes. The problem of elastic interaction in 3D solids is an old topic – though the reasoning we shall apply below has not been used so far. We shall concentrate on a 2D solid and thin films by considering that the defects are not necessarily isotropic (in that they do not induce a central force distribution).

It must be emphasized that a defect in a crystal induces in general by far no isotropic force distribution, although the elasticity of the solid may be treated as being isotropic (for example a 2D hexagonal solid obeys pure isotropic elasticity). Indeed, the defect interacts with the crystal locally in a fashion which detects the discrete nature of matter, that is totally anisotropic. As a consequence, the *defects do indeed interact linearly*, as will be shown.

## 6 Thin film theory

We consider here thin films. The ultimate limit is a very thin plate with an atomic thickness. In the absence of flexion (see section devoted to discussion), the displacement field is purely two dimensional in the plane ($x$, $y$). For a given force $\mathbf{f}\delta(\mathbf{r})$ the 2D-Lamé equation reads [19]:

$$\nabla^2\mathbf{u} + \frac{1+\sigma}{1-\sigma}\nabla(\nabla \cdot \mathbf{u}) = -2\frac{1+\sigma}{E}\mathbf{f}\delta(\mathbf{r})$$

by using the same method presented in [19] for the 3D case, we find the following 2D-displacement field:

$$\mathbf{u} = \frac{(1+\sigma)^2}{4\pi Eh}\left[\frac{\sigma-3}{1+\sigma}\mathbf{f}\ln(r) + \frac{\mathbf{r}(\mathbf{r}\cdot\mathbf{f})}{r^2}\right]. \tag{41}$$

In 2D we must substitute $Eh$ by $E_{2D}$ (the true 2D Young modulus). $E$ is the true bulk value and $h$ the film thickness. For an isotropic force distribution, we expect, in view of the discussion in Section 2, that the interaction law between two defects is $\sim 1/r^2$. However, as shown in the previous section the interaction energy vanishes exactly (in the sense of linear interaction). For an infinite

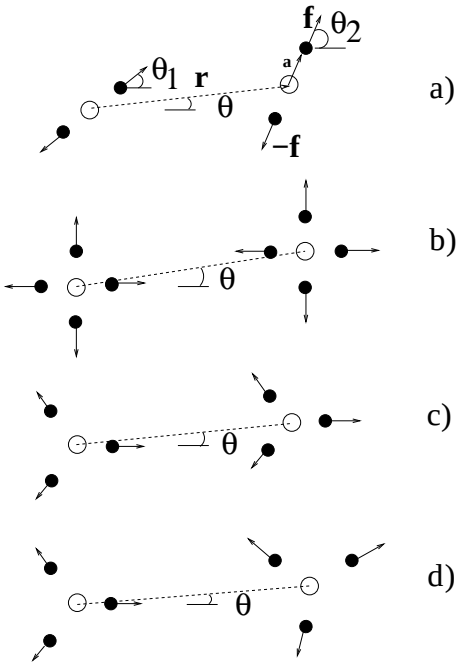


**Fig. 15.** Different kinds of force configurations: the geometry of forces is dictated by the defect symmetry.

system, and as stated before, there are two possibilities: either there is an induced interaction (see discussion), (ii) or that the defect symmetry is low enough. We shall consider different symmetries related to the defect. We focus here on the situation where the two defects are identical. As before, we represent a point defect as a set of concentrated forces $\mathbf{f}^{(n)}\delta(\mathbf{r}-\mathbf{r}^{(n)})$ confined in a area of a typical size $a$, ($|\mathbf{r}^{(n)}| < a$) and centered at the origin. Different symmetries are illustrated in Figure 15. The geometry of the force distribution around the defect is determined by the nature of the defect.

We consider the various geometries shown in Figure 15. For a 2D system, the displacement field $\mathbf{u}(\mathbf{r})$ created by a concentrated force $\mathbf{f}\delta(\mathbf{r})$ located at the origin is given by equation (41). On the other hand, for a finite thickness system, $\mathbf{u}(\mathbf{r})$ is defined by semi-infinite integrals which are listed in [21], which can be tabulated numerically (see Sect. 6.2).

### 6.1 Elastic interaction in 2D films

The evaluation of the interaction energy follows exactly the same procedure as in Section 4. That is, we first evaluate the response field due to a single force, and then sum up the contribution due to the whole set of forces corresponding to the symmetry under consideration. This step yields the total displacement due to the defect. Then using (16) we obtain the interaction energy. After expansion to leading order in the separation between the two defects we obtain the leading contribution. In the light of the previous sections the calculation is straightforward, we shall then only give the result:

$$F_{int} = \frac{(1+\sigma)f^2 g(\theta)a^n}{2\pi Ehr^n}, \tag{42}$$

where $g(\theta)$ is a function to be specified below, where $\theta$ represents the angle between the $x$ axis and the vector $\mathbf{r}$ (Fig. 15). Let us consider explicitly some examples:

(i) If the defect creates two opposite forces (Fig. 15a) the defect-defect interaction behaves as $\sim 1/r^2$ ($n = 2$), and it can be both attractive or repulsive depending on $\theta$,

$$g(\theta) = 2(1-\sigma)\left(\cos\left[2(\theta-\theta_1)\right] + \cos\left[2(\theta-\theta_2)\right]\right) + 2(1+\sigma)\cos\left[4\theta - 2(\theta_1+\theta_2)\right]. \tag{43}$$

(ii) For a four-fold symmetry (Fig. 15b) the leading non-vanishing contribution is $\sim 1/r^4$ ($n = 4$). In that case we obtain

$$g(\theta) = (25-5\sigma)\cos(4\theta). \tag{44}$$

Here also attraction and repulsion are both possible. Indeed the interaction is repulsive in the interval $-\pi/8 < \theta < \pi/8$, attractive for $\pi/8 < \theta < 3\pi/8$, and so on. Note that contrary to what could be expected from a dimensional analysis ($1/r^2$), this first contribution vanishes identically, due to the medium isotropy. If allowance is made for crystal anisotropy – that is, if the elasticity of the medium is anisotropic –, analytical results (like Eq. (41)) are not available. We have thus developed a numerical method to handle the anisotropic situation. We will outline the method in the next section.

(iii) For a three-fold symmetry (Figs. 15c-d), several situations can be encountered.

Firstly, if the two defects have the same orientation in space (Fig. 15c) (the geometry of the force configuration under consideration may occur in a hexagonal lattice; note that in 2D an hexagonal structure obeys exactly to isotropic elasticity) the interaction is found to be $\sim 1/r^4$ ($n = 4$). Here,

$$g(\theta) = -27\frac{(1+\sigma)}{2}\cos(6\theta). \tag{45}$$

The interaction is attractive in the sector $-\pi/12 < \theta < \pi/12$, repulsive when $\pi/12 < \theta < \pi/4$, and so on.

Another scenario may arise: this corresponds to the situation where the two defects have different orientations in space (Fig. 15d), in which case the interaction turns out to behave as $\sim 1/r^3$ ($n = 3$)

$$g(\theta) = 9\frac{(1-\sigma)}{4}\cos(3\theta). \tag{46}$$

The interaction is repulsive in the sector $-\pi/6 < \theta < \pi/6$, attractive for $\pi/6 < \theta < \pi/2$, and so on.

(iv) Let us quote another situation: suppose that one defect is isotropic, while the second is not. Suppose that the second defect has a two-fold symmetry (a force dipole making an angle $\theta$ with the line joining the two defects). By a similar procedure as in Section 5 (Eq. (35)), the displacement field due to a 2D isotropic defect is given by

$$\mathbf{u} = \frac{bf(1-\sigma^2)\mathbf{r}}{Ehr^2}, \tag{47}$$

where $b$ is the radius of action of the isotropic defect. Using (16) we obtain that the interaction energy is given to leading order by:

$$F_{int} = \frac{3}{2}\frac{f^2 ab(1-\sigma^2)}{Ehr^2}\cos(2\theta). \tag{48}$$

Of course, many other scenarii are possible, and they can be dealt with without additional complication. In the appendix we present another more general way for computing the elastic interaction by making use of the Green's function. Then many results will follow quite naturally depending on the symmetry associated with the defect.

Finally, if we consider any other higher symmetry, like 6-fold etc... we obtain an interaction law $\sim 1/r^n$ with $n = 6$, etc... However there exists another type of interaction, the induced one, which is of longer range, and it behaves as $1/r^4$. This interaction is akin to the induced interaction in electrostatics, and it is encountered when dealing with an interaction of an ion with a neutral atom [17]. The field created by an ion is given by $e/r^2$, where $e$ is the ion charge. The ion induces a polarization on the atom which is proportional to this field, leading thus to an interaction energy which behaves as $1/r^4$. We shall not give here the details of the calculation for the elastic problem which was studied in the past for a 3D solid. The idea there is that the elastic field of the first defect induces a local change of the forces (for example) associated with the second defect. Though the leading contribution between two isotropic defects is zero, the induced one is not. This interaction can also be called *nonlinear* [13]. We consider this question in Section 7.

### 6.2 Numerical results for anisotropic 2D films

For a full anisotropic elasticity a numerical analysis seemed necessary. We consider atoms in a lattice of a given crystal symmetry. Each atom is coupled to its nearest neighbors with a constant spring-like interaction. Let $\mathcal{M}$ denote the dynamical matrix associated with the oscillators, and $\mathbf{v}$ be the displacement vector of each atom ($\mathbf{v}$ has a dimension $2 \times N$, where $N$ refers to the number of atoms with two degrees of freedom each $(x,y)$). In the presence of two defects '1' and '2', $\phi_1$ and $\phi_2$ represent the potential energy of interaction between the defects and all the other atoms. The total energy in the harmonic approximation takes the form:

$$F = \frac{1}{2}\mathbf{v}^t \mathcal{M}\mathbf{v} + \phi_1 + \phi_2. \tag{49}$$

The above expression is equivalent to equation (10). The equilibrium value of the displacement is given by minimizing $F$ with respect to $\mathbf{v}$, which yields

$$\mathbf{v} = \mathcal{M}^{-1}\left(\mathbf{f}^{(1)} + \mathbf{f}^{(2)}\right) \tag{50}$$

where we have set $\mathbf{f}^{(i)} = -\partial\phi_i/\partial\mathbf{v}$, the force. Reporting into equation (49) and subtracting the contribution due to the defects as if they were alone, we obtain straightforwardly for the interaction energy $F_{int} = -1/2[\mathbf{f}^{(2)} \cdot \mathbf{v}^{(1)} + \mathbf{f}^{(1)} \cdot \mathbf{v}^{(2)}]$, which is the same expression as equation (16). We determine numerically the displacement field by inverting the matrix $\mathcal{M}$ (Eq. (50)). This method can be used for any anisotropy. Two important remarks have to be made. Firstly, $\mathcal{M}$ has to be inverted after projecting the vectorial space of displacement into subspace orthogonal to any degenerate modes. Secondly, periodic boundary conditions have to be considered in order to take advantage of the translational invariance of $\mathcal{M}$ and calculate its inverse on the plane wave basis. Inversion of $\mathcal{M}$ in the case of a square lattice has led to the following results.

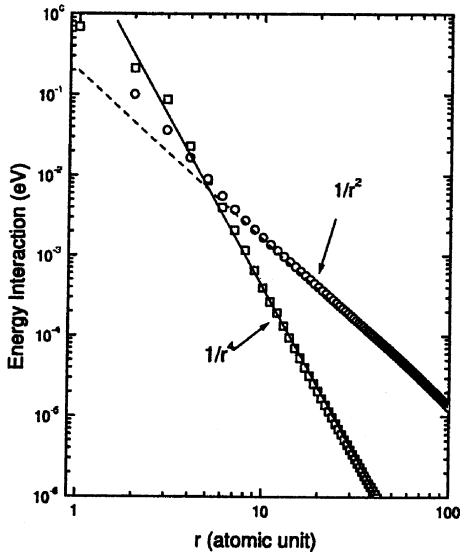


**Fig. 16.** Interaction energy between defects with a four-fold symmetry (Fig. 14b). Comparison between isotropic (squares) and non-isotropic (circles) elastic 2D layer. Solid and dashed lines allow one to estimate deviation from power law. Isotropic case: $C_{11} = 2.333 \times 10^{11}$ Pa, $C_{12} = 10^{11}$ Pa and $C_{44} = 0.666 \times 10^{11}$ Pa. Anisotropic case: $C_{11} = 1.680 \times 10^{11}$ Pa, $C_{12} = 1.210 \times 10^{11}$ Pa and $C_{44} = 0.75 \times 10^{11}$ Pa (Cu values).

(i) If the dynamical matrix is taken to be that of an isotropic medium we find the above-mentioned $\sim 1/r^4$ for a four fold force distribution (Fig. 16). We can check that continuum theory gives reliable results with a cutoff of about three or four atomic distances $a$. In addition, below this distance, chemical interactions should prevail on elastic interactions. Therefore, the discrepancy between continuum and discrete theory below this cutoff is of minor importance. This result seems to be confirmed by preliminary *ab initio* calculation [22].

(ii) If $\mathcal{M}$ is taken to be fully anisotropic, then we find for the four fold distribution that the leading contribution is $\sim 1/r^2$ (instead of $\sim 1/r^4$). Here attraction and repulsion are both possible. Figure 16 also shows the $r$-dependence of 2D elastic interaction in isotropic ($\sim 1/r^4$) and anisotropic ($\sim 1/r^2$) media. This difference is explained by the cancellation of the lowest order term of the dipolar expansion in the case of an isotropic medium, while these terms do not cancel for a

**Table 1.** Summary of different elastic interactions that can be encountered. Superscripts c and d refer to Figures 15c and 15d respectively.

| Point defect | semi-infinite | 2D |
|---|---|---|
| dipole (2-fold) | $+1/r^3$ | $\pm 1/r^2$ |
| 3-fold [c] | $+1/r^3$ | $\pm 1/r^3$ |
| 3-fold [d] | $+1/r^3$ | $\pm 1/r^4$ |
| 4-fold | $+1/r^3$ | $\pm 1/r^4$ |
| isotropic defect | $+1/r^3$ | 0 |
| step-step dipoles | $1/r^2$ | 0 |
| step-step mono-poles | $\ln(r)$ | $r$ |

non-isotropic medium. Table 1 summarizes the different possible interactions for a semi-infinite and a 2D solid.

### 6.3 Numerical results for film with finite thickness, comparison with 2D and 3D limits

Let us finally discuss the situation where the film has a finite thickness. The question thus arises of to what extent interaction laws in a thin film, but of finite thickness, would produce the semi-infinite limit or 2D limit. Qualitatively we expect that if defects inter-distance is large in comparison to the film thickness, then the interaction should be effectively of 2D nature. Conversely for short separations in comparison to the thickness, a semi-infinite behaviour should prevail. Evaluation of the elastic field in a semi-explicit form (in a form of integrals that we have tabulated) created by a localized force at the surface of a thin film are known and are listed in [21]. Using that field it is possible to evaluate numerically the defect-defect interaction by using the definition of the interaction energy (Eq. (16)). We find that at $r/h \ll 1$ the interaction is repulsive and is given by $\sim 1/r^3$, as expected. At larger separation ($r/h \gg 1$), we recover the above-discussed 2D interaction. If the orientation in 2D is such that the interaction is attractive ($\theta = \pi/4$ ), the full interaction exhibits a minimum at $r \sim h$ as shown in Figure 17. The order of magnitude for a concentrated force is chosen in the case of epitaxial crystal growth. Considering that $f = (\Delta a/a)Ea^2/(1-\sigma^2)$ where $\Delta a/a$ is the layer deformation typically equal to 5% in the case of Si/Ge system, $a \approx 5$ Å, $E \approx 10^{11}$ Pa and $\sigma \approx 0.3$ lead to $f \approx 10^{-9}$ N, this value is also confirmed by *ab initio* calculations [22].

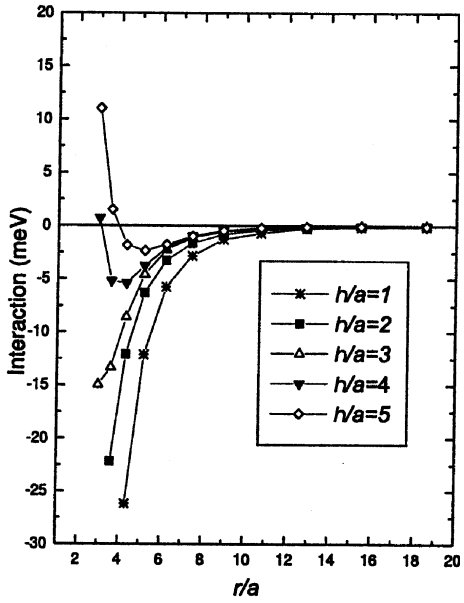


**Fig. 17.** Elastic interaction in the case of a four-fold symmetry (Fig. 9b) for different layer thicknesses. $f \approx 3\times 10^{-9}$ N, $\sigma \approx 0.3$ and $E \approx 3 \times 10^{11}$ Pa (typical silicon values).

## 7 Discussion

This section is devoted to discussions of the main implications of our results and to some comments about the problem of the induced interaction, and the contribution of the flexion of thin films.

The first question we address here is how can one extend the results to non point defects from the knowledge of point defects contributions. Let us first consider the case of a step or linear defects in 2D and thin films. Steps, or chain of atoms on a thin film, are locations of force dipoles [23]. In order to evaluate the field due to a step, we integrate over one of the two chains from $-\infty$ to $+\infty$. For a defect at a surface of a 3D, the interaction between two point defects behaves as $\sim 1/r^3$ (see Eq. (32)). This leads to the well known line-line $\sim 1/\ell^2$ ($\ell$ = line-line distance) interaction by integrating this law along one line. When the linear defect is an edge lying at the junction between two different kinds of materials or crystalline structure (hetero-epitaxy, or anisotropy), then the defect is a location of force mono-poles $\mathbf{f}$ [23,24] and one needs to integrate the law $\sim 1/r^3$ over one domain and then along the edge, so that the resulting edge-edge interaction is $\ln(\ell)$. In 2D, very different behaviours occur. As seen in this paper (Sect. 6) a dipole in 2D creates a displacement field behaving as $\sim 1/r$, thus we find that the interaction energy between two linear defects vanishes identically, since it involves the combination $[u_s(\ell+a)-u_s(\ell-a)]f$ where $u_s$ is the displacement due to the step – from equation (41) $u_s$ is found as being independent of the distance and $\ell$ is the inter-step distance. In contrast, when the edge is a location of force mono-poles $\mathbf{f}$ (this holds also in general if the surface stress tensor is anisotropic; that is if its values on both sides of the linear defect are different), we find, upon integration of $\mathbf{u}$ along the line, the displacement due to a step. Multiplying by the force $\mathbf{f}$ and integrating over a unit length leads to the edge-edge interaction energy:

$$F_{int} = -\frac{\lambda(1-\sigma^2)}{2Eh} f^2 \ell \qquad (51)$$

where $\lambda$ is the linear density of mono-poles. This interaction is attractive if the two mono-poles are anti-parallel, and repulsive otherwise. This result differs from the classical law $\ln(\ell)$ encountered for a semi-infinite medium. The present interaction is much stronger.

Another important implication concerns the quantum dots fabrication. It is still a puzzling question to determine precisely how and by which mechanism island organization [2] takes place. A moving atom (say during growth and nucleation) would follow a path of attraction until it reaches another atom or island. Thus one would expect clustering to be enhanced along attractive directions, and reduced along repulsive ones. Numerical Monte Carlo simulations [25] reveals an influence of elastic effects on island morphology and density. If the system has a finite thickness $h$ (as is often the case in the production of nanostructures) repulsion is found at shorter distances and clustering may become prohibited. More precisely, suppose that an island of some size has formed during growth. Other islands may form by random nucleation, and a size distribution takes place, even in the absence of elasticity [26]. The distribution is a result of nucleation and competition of islands for the same diffusion field. What would happen in the presence of elasticity? When an island forms, it creates an elastic field, and its interaction with an isolated adatom increases with its size. If elementary interaction is of 2D nature, defects on the mono-layers should lead to interactions of the nature presented here. Several scenarii may occur depending on the specific problem under consideration (nature of defects, symmetries...). We shall not address these questions in this paper; the results presented here should serve as a basis for a more precise discussion.

Let us now turn to the question of experimental testability of our theory. It is still challenging to have a direct test of elementary interactions on the atomic scale. However, indirect tests similar to those developed for thick solids can be achieved [27]. For example, the study of the step fluctuation spectrum on a vicinal surface can give a direct access to a measure of the elastic interactions. For a very thin film the same analysis may be performed to check the dependence of the spectrum of supported thin films having steps. One can also conceive of simple macroscopic systems, like large 2D elastic sheets in which one inserts defects (like small elongated disks, having different types of symmetries; 2 folds, 3 folds, etc...) that distort the sheet. A second disk sitting in the neighborhood would feel a displacement. The force that is needed to keep it at the same point should give direct information on the elastic interactions. If the elastic sheet is optically transparent, use of photoelasticity should allow a direct visualization access to the elastic field. We hope that these kinds of experiments will be performed in future.

We have seen that two isotropic defects in unbounded systems and in any dimension do not interact linearly. There is an interaction energy which is induced and this behaves as $1/r^4$ in all cases. Like in electrostatics, an ion and a neutral atom with spherical symmetry do not interact to leading order, but the ion induces a polarizability on the atom leading to an interaction which is the product of the polarizability (which is proportional to the field of the ion) times the field of the ion. Since the last one is $\sim 1/r^2$ the interaction is $\sim 1/r^4$. Here the situation, albeit a bit more complex, is conceptually similar. The presence of the first defect causes a change of some quantity related to the second defect (like the polarizability of the atom). A natural quantity characterizing the defect is the set of forces (or energy) of reaction of the material. The defect has a bare force $f_0$, plus a force caused by the presence of the other defect, which is, to leading order, proportional to the deformation caused by it ($f_1 u_0$, $u_0$ is the displacement caused by $f_0$ of the first defect), to leading order. Since the displacement $u_0 \sim f_0/r$ (in 2D) (this is the contribution of a dipole), and because the total force must be zero on the second defect, one has to multiply the field of the first defect $u_0$, by $f_0(1 + f_1/f_0 u_0')$ (the prime is differentiation with respect to $r$), and then differentiate the product with respect to $r$, since the second defect is represented by a set of forces whose sum is zero.

The interaction has thus the form

$$F_{induced} \sim [f_0 u_0 (1 + (f_1/f_0) u_0')]'. \tag{52}$$

Since the contribution coming from $f_0$ (non-induced) vanishes according to the result of Section 5, one finally has

$$F_{induced} \sim f_1 (u_0 u_0')'/f_0 \sim \frac{f_1 f_0^2}{r^4}. \tag{53}$$

Very much like in electrostatics the same law holds here but with a spatial dimension which is equal to 2, here, and 3 in electrostatics [17] (that both laws have the same power law despite the difference in the spatial dimension is simply due to the fact that in elasticity there is no 'net charge'). The same reasoning applied to 3D leads to an induced interaction $\sim 1/r^6$.

Finally, let us address another question of major importance in several circumstances. For thin films or 2D systems buckling may become important. More precisely, which among the two following interactions would dominate: the one stemming from elastic deformation in the plane – as studied here –, or rather the out-of plane (plate flexion) one? Let us evaluate the flexion contribution. Let $\zeta(x, y)$ denote the flexion profile counted from a plane configuration. In the presence of a localized force $f\delta(\mathbf{r})$, $\zeta$ obeys the bi-harmonic equation [19]

$$\kappa \triangle^2 \zeta = f\delta(\mathbf{r}) \tag{54}$$

where $\kappa = Eh^3/12(1-\sigma^2)$ is the film bending rigidity, and $h$ the film thickness. Let us consider a defect which enjoys the spherical symmetry. The solution is [28]

$$\zeta(\mathbf{r}) \sim f \frac{1}{16\pi\kappa} r^2 \ln(r). \tag{55}$$

This could also be inferred from dimensional considerations: the solution to the Poisson equation in 2D is $\ln(r)$, and since $\zeta$ obeys a bi-Laplacian equation, one has to integrate twice with respect to $r$. Since a defect corresponds to a set of forces with both the total force and torque being zero, it must be represented by three forces at least (like the one represented in Fig. 3a) $f$ at $-a$, $f$ at $a$ and $-2f$ at 0. Thus the total field created by the defect $\zeta_T \sim \partial^2\zeta/\partial r^2$ is dimensionally given by

$$\zeta(\mathbf{r}) \sim f a^2 \frac{1}{16\pi\kappa} \ln(r). \tag{56}$$

The interaction energy with a second defect located at $r$ implies an additional second derivative (since one has to multiply $\zeta_T$ by each force: by $f$ at $r-a$, $f$ at $r+a$ and $-2f$ at $r$), so that the interaction energy $F_{flex}$ is given by

$$F_{flex} \sim (fa)^2 a^2 \frac{1}{16\pi\kappa r^2} \sim \frac{(fa)^2 a^2}{\pi E h^3 r^2}. \tag{57}$$

From the analysis of Section 6 we have obtained that dipole-like defects obey the following in-plane interaction law

$$F_{int} \sim \frac{(fa)^2}{2\pi E h r^2}. \tag{58}$$

Comparison of the above expressions shows that the interaction *via* flexion may become comparable to that induced by in-plane deformations if $h \sim a$ (while for films with few atomic thicknesses or wider, the in-plane interaction prevails). Of course numerical factors of order unity have been disregarded, and a precise evaluation requires a more quantitative study. Suffice it to say here that for atomic films the question of interaction *via* flexion must be looked at under close scrutiny.

## Appendix

The aim of this appendix is to provide the interaction energy in terms of a general expression by using the Green's function associated with the elastic field in an unlimited medium (3D or 2D).

Starting from equation (16) and considering two identical defects A and B (Fig. 5), we get:

$$F_{int} = -\sum_m f_i^{(m)}\, u_i^{(m)}, \tag{59}$$

where the subscript $i$ represents $x$, $y$ or $z$. The displacement $u_i^{(m)}$ can be written as:

$$u_i^{(m)} = u_i\left[\mathbf{r} + \mathbf{a}^{(m)}\right]$$

considering that each defect applies forces on its nearest neighbors, *i.e.* at short distances ($a$) in comparison to the inter-defect distance ($r$), we can expand $u_i[\mathbf{r} + \mathbf{a}^{(m)}]$ about $\mathbf{r}$:

$$u_i\left[\mathbf{r} + \mathbf{a}^{(m)}\right] = u_i(\mathbf{r}) + a_j^{(m)} \partial_j u_i(\mathbf{r}) + ...$$

Thus, equation (59) becomes to first order:

$$F_{int} \approx -\left[D_i\, u_i + D_{ij}\, u_{ij}\right] \tag{60}$$

where:

$$\begin{cases} D_i = \sum_m f_i^{(m)} = 0 \\ D_{ij} = \sum_m f_i^{(m)}\, a_j^{(m)} \text{ and } u_{ij} = \partial_j u_i \end{cases} \tag{61}$$

$u_i(\mathbf{r})$ is the displacement at point $\mathbf{r}$ created by the forces applied by defect A. Thus, it can be written as:

$$u_i(\mathbf{r}) = \sum_n u_i^{(n)}\left[\mathbf{r} - \mathbf{a}^{(n)}\right] \tag{62}$$

where $u_i^{(n)}\left[\mathbf{r} - \mathbf{a}^{(n)}\right]$ is the displacement at the distance $\mathbf{r} - \mathbf{a}^{(n)}$ from the localized force $\mathbf{f}^{(n)}$ (that creates $\mathbf{u}^{(n)}$) belonging to defect $A$ and applied at $\mathbf{a}^{(n)}$. Then, expanding $u_i^{(n)}[\mathbf{r} - \mathbf{a}^{(n)}]$ about $\mathbf{r}$, we obtain:

$$u_i^{(n)}[\mathbf{r} - \mathbf{a}^{(n)}] = u_i^{(n)}(\mathbf{r}) - a_k^{(n)} \partial_k u_i^{(n)}(\mathbf{r}) + ... \tag{63}$$

where $u_i^{(n)}(\mathbf{r})$ is the displacement at distance $\mathbf{r}$ from a localized force $\mathbf{f}^{(n)}$ applied at the origin. Using the Green's function $G_{il}$ which is defined as:

$$u_i^{(n)}(\mathbf{r}) = G_{il} f_l^{(n)}, \tag{64}$$

equation (63) can be rewritten as:

$$u_i^{(n)}\left[\mathbf{r} - \mathbf{a}^{(n)}\right] = G_{il}(\mathbf{r})\, f_l^{(n)} - a_k^{(n)} \partial_k G_{il}(\mathbf{r})\, f_l^{(n)} + ... \tag{65}$$

Then using (60, 61, 62) and (65) we get:

$$F_{int} = D_{ij}\, D_{lk} \partial_j \partial_k G_{il}(\mathbf{r}) \tag{66}$$

where $D_{lk} = \sum_n f_l^{(n)}\, a_k^{(n)}$. Again, we have used the mechanical equilibrium condition, *i.e.* $\sum_n f_l^{(n)} = 0$. For simplicity we consider identical defects (thus the same tensor $D_{lk}$ occurs twice). Expansion to higher orders is straightforward.

Equation (66) allows one to derive directly the elastic interaction by using the expression of the Green's function along with the symmetries associated with the defect. For example, for an isotropic defect, we have $D_{ij} = A\delta_{ij}$ where $A$ is a scalar. Then using equation (66), we obtain:

$$F_{int} = A^2 \partial_{ii} G_{ii}(\mathbf{r}) = A^2 \Delta G(\mathbf{r}), \tag{67}$$

where we have used the fact that $G_{xx} = G_{yy} = G_{zz} = G$ (isotropy). In 3D the Green's function is given by the following expression [19]:

$$G_{ik} = \frac{1}{4\pi\mu}\left[\frac{\delta_{ik}}{r} - \frac{1}{4(1-\sigma)} \frac{\partial^2}{\partial x_i \partial x_k}\, r\right] \tag{68}$$

$\mu = E/2(1+\sigma)$ is the shear modulus. It is easily checked that $\Delta G = 0$, and finally $F_{int} = 0$. Thus two isotropic defects in an unlimited medium do not interact linearly, as we have seen in Section 5. Note that the expression given by (67) is an expansion to the leading order in $a/r$. If one expands to higher orders we simply generate derivatives of $\Delta G$, which vanish, obviously. The same reasoning in 2D (the corresponding Green's function is inferred from equation (41) (or in any dimension) leads to the same conclusion.

Imagine now two anisotropic defects like the two force dipoles represented in Figure 6, the first dipole makes an

angle $\theta_1$ with the $x$-axis while the second dipole makes an angle $\theta_2$; the line joining the two defects makes an angle $\theta$. The generic form of the tensor $D_{ij}$ is

$$D_{ij} = A\delta_{ij} + B\left(n_i n_j - \frac{1}{2}\right), \tag{69}$$

where $\mathbf{n}$ is the unit vector pointing along the dipole. Here, we have $A = fa$, $B = 2fa$, $n_x = \cos(\theta_1)$ and $n_y = \sin(\theta_1)$, and similar expressions for the second defect. The Green's function in the 2D case is given by

$$G_{ij} = \frac{(1+\sigma)^2}{4\pi Eh}\left[\frac{\sigma-3}{1+\sigma}\ln(r) + \frac{x_i x_j}{r^2}\right]\cdot \tag{70}$$

After some algebra, expression (66) gives:

$$F_{int} = \frac{a^2 f^2(1+\sigma)}{2\pi Ehr^2} g(\theta,\theta_1,\theta_2), \tag{71}$$

with

$$\begin{aligned} g(\theta,\theta_1,\theta_2) = {} & 2(1-\sigma)\left(\cos\left[2(\theta-\theta_1)\right] + \cos\left[2(\theta-\theta_2)\right]\right) \\ & + 2(1+\sigma)\cos\left[4\theta - 2(\theta_1+\theta_2)\right] \end{aligned} \tag{72}$$

which is exactly the same expression as equation (43) (Sect. 7). If the defect is not of a two-fold symmetry (for example if it enjoys the $C_3$ symmetry) then $B = 0$ and one has to expand (63) to next order generating thus an interaction which has a form (by analogy with (66)) where the general term being $F_{int} \sim D_{ml} T_{ijk} \partial_{jkl} G_{im}$. The third order tensor $T$ has in general the following form

$$T_{ijk} = \sum_n f_i^{(n)} a_j^{(n)} a_k^{(n)}. \tag{73}$$

Exploitation of this expression leads to the same law for the three-fold symmetry discussed in Section 6.

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28. As shown in [13] the interaction energy between two isotropic defects which is mediated by flexion vanishes exactly in the linear regime. If one defect is anisotropic then the interaction is $\sim 1/r^2$ and the present argument is still qualitatively correct