Topological Defects in Crystals

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Abstract
In this seminar an introduction to topological defects and the theory used to describe them is presented. Specifically we focus on dislocation defects and defects in vectorial order parameter fields that appear in various materials. Examples include materials that can be modeled as a lattice of spins, smectic liquid crystals, solid crystals and superfluid $^4$He. In this materials we introduce topological invariants such as winding number, topological charge and Burgers vectors. Some effects of the defects on physical properties of matter are explained.
1 Introduction

A topological defect is in general characterized by some core region (e.g., a point or a line) where order is destroyed, and a far field region where an elastic variable changes slowly in space. Like an electric point charge, it has the property that its presence can be determined by measurements of an appropriate field on any surface enclosing its core [1, p. 495]. Depending on the material and the symmetry that is broken, different defects are possible. A few examples are shown in Figure 1. On all images the singularity in which the order parameter is discontinuous (at the center of the defect) is visible.

Figure 1: Examples of defects: (a) vortex in 2D xy-model, (b) “hedgehog” in 3D space with 3D unit spin, (c) +90° twist in a solid crystal [1].

Topological defects describe distortions in the system’s order, that can be observed even from distances, far away from the defect itself. These defects introduce changes into the crystal’s lattice, and as opposed to the effects of doping, the changes in the crystal’s lattice are not local and cannot be isolated. We can use this theory to describe very abstract changes in system’s order (Figure 1) (a) formation of vortices in 2D models with 2D spins, (b) “hedgehog” defects that appear in 3D spin models and even (c) defects in crystal lattice that break the rotational symmetry in 3D solids.

The symmetry of some defects is hard to understand intuitively; therefore, a formal language for its description is even more necessary. Homotopy theory [2] provides such formal language, and in this
seminar an introduction into what it can offer is given. 
Topological defects are important in understanding properties of various materials, including solid crystals [1], liquid crystal colloids [3] and even formation of vortices in superfluid 4He [4]. In solid crystals the importance is such, that models that do not take into account the effects of topological defects give incorrect predictions of yield stress off by an order of magnitude. Crystal growth is also significantly affected. In liquid crystal colloids the defect lines crucially determine the configuration of colloids. Therefore finding methods for controlling the defects is particularly important.

This seminar is organized as follows: Chapter 2 presents a simple system in which topological defects occur. Categorization of defects is described, and an explanation of the reasons for existence of such defects, based on the studied example is given. A combination of defects and defect interactions are presented. Chapter 3 presents an overview of topological defects in different media, such as smectic liquid crystals and solid crystals, and Chapter 4 describes effects of defects on physical properties of materials.

2 An illustrative example: 2D spins in 2D lattice

2.1 Order parameter

Topological defects are entities with order parameter fields of various materials. Order parameters are typically spatial (and also temporal) fields in various dimensions. They can be scalar fields, vector fields or even tensor fields. Here a system of 2D spins in 2D lattice is presented. The spins in this system can be described as a vector in a plane. We define the order parameter as

\[ \vec{s} = (\cos(\theta(\vec{r})), \sin(\theta(\vec{r})))] \]

where \( \theta(\vec{r}) \) defines the direction of the field [2]. \( \theta \) uniquely defines \( \vec{s} \) and can therefore be used as an order parameter as well. It is convenient to introduce a concept of order parameter space \( \mathcal{M} \). For 2D unit length spins, this is the unit circle \( S_1 \), for 3D unit length spins this is the surface of the unit sphere \( S_2 \), and for n-component spins, this is the surface of a \( n-1 \) dimensional sphere \( S_{n-1} \). The subscript indicates the dimensionality of the sphere itself, and not the dimensionality of the space in which the sphere is embedded.

It is also convenient to define \( \mathcal{D} \) as coordinate space domain (in the case of 2D spins in 2D lattice, this is 2D space) and \( \Gamma \) as a closed loop in \( \mathcal{D} \). In our example, specification of \( \theta \) on \( \Gamma \) defines a mapping from the loop \( \Gamma \) in coordinate space domain \( \mathcal{D} \) into the unit circle \( \mathcal{M} = S_1 \). A visualization of this mapping is shown in Figure 2.

Even if this simple example seems distanced from real materials, we obtain the same order parameter space in the case of superfluid 4He [2] where the order parameter is a complex scalar field of fixed magnitude but arbitrary phase:

\[ \psi(\vec{r}) = \psi_0 e^{i\theta(\vec{r})} \]

\( \psi \) is the wave function of superfluid 4He. As the order parameter spaces are equal, all topological defects can be described in the same way even though the observed systems are very different.

2.2 Categorization of defects

To formalize the description of topological defects, we must determine which defects are similar enough that they could be classified as topologically equivalent. It is expected that two mappings, which can be continuously deformed in such a way that they become equal, should describe the same topological defect. If such continuous deformation cannot be found, the defects must be classified as different. Figure 3 shows three examples of different mappings. In Figure 3 (a) all the spins point to the same direction, therefore the entire loop is mapped into one point in \( S_1 \), and the position of the point on the unit circle corresponds to the direction in which the spins are ordered. Figure 3 (b) shows a mapping that can be deformed into the first mapping by continuous deformation, therefore the defects (a) and (b) are instances of the same topological defect. In Figure 3 (c) presents a mapping that cannot be deformed into a point like the first two mappings as this mapping wraps the unit circle twice. In this way we can classify the

\(^{1}\)Order parameter of a unit length was chosen for reasons of simplicity. We could take the strength of the ordering into account as well (as in [1]), but this would make the order parameter space two dimensional and not allow us to draw simple diagrams of this space.
**Figure 2:** Example of a mapping from the loop $\Gamma$ in coordinate space domain $\mathcal{D}$ into the unit circle $\mathcal{M} = S^1$ [1].

**Figure 3:** An example of different mappings: figures (a) and (b) show different mappings of the same topological defect. Figure (c) shows a mapping of a different topological defect [2].

**Figure 4:** Figures (a) and (b) show two vortices with winding number $k = 1$. From figure (c) it is evident that a continuous transformation from (a) into (b) is possible [2].

defects into different homotopy classes. In our 2D model we can classify defects according to their winding number, that is the number of times their mapping wraps $S^1$ ($\Gamma$ encircles the defect in counterclockwise direction).

In our example space, we can formally define the winding number with the following integral:

$$\oint \frac{d\theta}{ds} ds = 2k\pi$$

where the integration around the core is taken in counterclockwise direction. The sign of the winding number corresponds to the direction in which the mapping wraps the order parameter space; for negative values of $k$ the order parameter space is wrapped in the opposite direction as the corresponding path around the core. The mappings (a) and (b) in Figure 3 have winding number $k = 0$, and mapping (c) has winding number $k = 2$. In Figure 4 we show a few defects that appear different, but have the same winding number. Figures (a) and (b) show two vortices with winding number $k = 1$. It is evident from Figure (c) that one can transform one of the vortices into another by a continuous distortion, as the vortex in (c) resembles (a) in its center, and then continuously transforms into the configuration (b). Figure 5 shows defects with different winding numbers. The directions of the arrows show the directions of the spins at a given point in space. Removal of a singularity by continuously deforming a region of space is shown in Figure 6. The region where the direction of order parameter rapidly changes can be continuously transformed into a region where all changes in the direction of the order parameter are continuous. Because this is possible, we know that both configurations have a winding number $k = 0$ (as only singularities with winding number 0 can be removed).
2.3 Defect interactions

The integral definition of the winding number accounts also for a combination of defects. If we want to study the combined effect of several vortices, we can imagine a sequence of continuous distortions that deform $\Gamma_1$ and $\Gamma_2$ into one continuous loop (see Figure 7). If such a sequence of continuous deformations exist, we can use the integral definition of a winding number for the combined path and see that the effective winding number of a system of vortices is the sum of the winding numbers of all components (this relies on the fact that the order parameter change on path from the first defect to the second defect cancels the change on the path in the opposite direction - for complicated order parameters this might not be true).

A net effect of two vortices with opposite winding numbers on the far-field can be seen in Figure 8. On figures (a) and (b) a combination of two vortices with winding numbers $k = +1$ and $k = -1$ is shown. We can see that the net effect of both vortices is zero and the far field is not affected by this combination of vortices in the first order of approximation [1].

An example of the addition rule is shown on figures (c) and (d). Two vortices with winding numbers $k = +1$ are shown on figure (c), and on figure (d) one vortex with $k = +2$ is shown. We can see that topologically, the far field is equivalent. [2].

![Figure 5: Defects with different winding numbers $k$ [2].](image)

![Figure 6: Removal of a singularity by a continuous deformation [2].](image)

![Figure 7: Combining two vortices [1].](image)

2.4 Energies of vortices in 2D spin systems

The energy of vortices consists of two parts: (1) the core energy $E_c$ and (2) the elastic energy $E_{el}$. The core energy is associated with destruction of the order parameter at the core of the defect, and requires a microscopic order model for precise calculation. A good estimate of $E_c$ can be made by observing that the increase in free energy per unit volume due to the destruction of the order parameter is the condensation energy density $f_{cond}$ of the ordered state. The core energy is thus of order of magnitude of the area (or volume) of the defect

$$E_c = Aa^2 f_{cond}$$

where $A$ is a numerical constant, $a$ is the radius of the defect.

To calculate the elastic energy contribution, we must evaluate the energy cost of the slow spatial variation
Figure 8: Examples of combined effects of vortices (a) and (b) [1]. (c) and (d) [2].

of the elastic variable in the field far from the defect. In case of a 2D vortex with winding number \( k \) from the first example, the constraints that the elastic variable must meet are

\[
\int d\Theta = 2k\pi
\]

\[
\frac{\delta F_{el}}{\delta \Theta(\vec{r})} = -\rho_s \nabla^2 \Theta(\vec{r}) = 0
\]

where \( \rho_s \) is spin-wave stiffness or rigidity measured in units of energy/length\(^{d-2} \) (\( d = 2 \) in this case) and the absence of external field is taken into account in the equation 8 \( (F_{el} = 0) \). We integrate the elastic energy density caused by the field

\[
\Theta = k\Phi
\]

\[
\nabla \Theta = \frac{k}{r} \hat{\theta}
\]

which satisfies both constraints \( (r^2 = x^2 + y^2) \) in the entire sample.

The integration gives

\[
E_{el} = \frac{1}{2} \rho_s \int d^2 \vec{r} [\nabla \Theta(\vec{r})]^2
\]

\[
= \frac{1}{2} \rho_s 2\pi k^2 \int_0^R \frac{r dr}{r^2}
\]

\[
= \pi k^2 \rho_s \ln(R/a)
\]

where \( R \) is the linear dimension of the sample. We can obtain the core radius by minimizing the total energy \( E_0 = E_c + E_{el} \) (zero of derivative):

\[
0 = -\frac{\pi k^2 \rho_s}{a} + 2a A f_{cond}
\]

\[
a^2 = \frac{\pi k^2 \rho_s}{2 A f_{cond}} \sim k^2 \xi^2
\]

where we used Josephson scaling relation \( \rho_s \sim T_c \xi^{-2} \) and \( f_{cond} \sim T_c \xi^{-d} \) (equation 6.1.11 from Principles of condensed matter physics [1]). Core radius \( a \) is therefore proportional to correlation length \( \xi \). The core energy at optimal \( a \) grows quadratically with \( k \):

\[
E_c = \pi \rho_s k^2 / 2
\]

The calculation in 3D is the same, the only difference is that in this case the calculated core energy is the energy of the core per unit length of the vortex line.
2.5 Combining defects

To calculate the combined energy of two vortices we must use a different approach. The plane in which the vortices lie is cut two times, along the $x^+$ and $x^-$ axes so that the area between the vortices is left uncut (see Figure 9). The two surfaces of each cut are labeled $\Sigma^+_1$ and $\Sigma^-_1$ and their normals are $+\vec{e}_\phi$ and $-\vec{e}_\phi$. We obtain the vortex energy by integration per parts, using the fact that $\nabla^2 \Theta_{1,2} = 0$ and introducing the variables $\vec{v}_s = \nabla \Theta$ and $\vec{h}_s = \rho_s \vec{v}_s$:

$$E_{cl} = \frac{1}{2} \rho_s \int d^2 \vec{r} [\vec{v}_s^{(1)} + \vec{v}_s^{(2)}]^2$$

$$= E_1 + E_2 + \frac{1}{2} \int d^2 \vec{r} [\vec{h}_s^{(1)} \vec{v}_s^{(2)} + \vec{h}_s^{(2)} \vec{v}_s^{(1)}]$$

$$= E_1 + E_2 + \frac{1}{2} (\Theta^+_2 - \Theta^-_2) \int_\Omega \rho_s \frac{k_1}{r} dr + \frac{1}{2} (\Theta^+_1 - \Theta^-_1) \int_\Omega \rho_s \frac{k_2}{r} dr$$

$$= E_1 + E_2 + 2\pi \rho_s k_1 k_2 \ln(R/r)$$

where $E_1$ and $E_2$ are energies of two combined vortices that are $r$ apart. If we use the result in Equation 11, we get:

$$E_{cl} = \rho_s \pi (k_1 + k_2)^2 \ln(R/a) + 2\pi \rho_s k_1 k_2 \ln(a/r)$$

which allows us to draw some conclusions about a system of vortices:

- $\ln(R)$ divergence disappears if $k_1 = -k_2$, or for a system of more than two vortices where $\Sigma k_i = 0$. This means that for such a system the far field is not changed in any way - from far away, this system is undetectable.

- Sign of the interaction depends on relative signs of $k_1$ and $k_2$. As $\ln(a/r)$ is a monotonically decreasing function of $r$, this means that two vortices of the same sign will repel each other and two vortices of opposite signs will attract each other.

We can also calculate the force $F_{21}$ exerted by vortex 1 on vortex 2:

$$F_{21} = -\nabla_2 E = 2\pi \rho_s k_1 k_2 \frac{\vec{r}_2 - \vec{r}_1}{|\vec{r}_2 - \vec{r}_1|^2}$$

2.6 Physical stability of topological defects

According to the definition, topologically distinct defects cannot be transformed into different topological defects with a transformation that continuously changes the order parameter. We can interpret this as if there was an infinite energy barrier stopping this process (in reality this barrier is always finite, but of very different magnitude depending on the system). For example, if the defect with $k = 1$ was to be removed, the continuous transformation would have to go either through a state with two boundaries as shown in Figure 10, or through an isotropic phase. The energy of the state shown in Figure 10 (a) is of order $J \ln(L)$, where $J$ is the exchange energy and $L$ is the size of the sample. This estimate is made by following equation 11 $E_{cl} = \pi k^2 \rho_s \ln(R/a)$ taking into account that $\rho_s$ is a linear function of the exchange energy $\rho_s \approx J$ and $R$ is the linear dimension of the sample ($R = L$). The energy of the state where boundaries are formed as shown in Figure 10 (b) is much higher (order of magnitude $J L^2$ - energy is a linear function of the size of the boundary which in turn scales as $L$ in 2D), so the probability of this process is very low and in practice, this process does not occur. The energy barrier of a transition through an isotropic phase is even higher, of order $J L^2$ and therefore even less probable.
2.7 Topological stability of defects

In order to study topological stability it is convenient to define a quantity called \textit{codimension} as

\[ d' = d - d_s \]  

(21)

where \( d \) is \textit{dimensionality of space} in which the defect appears, \( d_s \) is the \textit{dimensionality of the core of defect}, and for further reference it is also useful to define \textit{dimensionality of order parameter space} as \( n \).

We can say that codimension represents the number of free dimensions in a region in which the order parameter may change. The only possibility for a topologically stable defect with continuous change of the order parameter around the core is \( d' = n \) \cite{1}. In our example of vortices in 2D space, \( d = 2 \), \( n = 2 \) and \( d_s = 0 \) which satisfy the equality.

If \( d' < n \) there are no topologically stable defects. The defect can always escape to at least one “leftover” dimension. In Figure 11, a point defect \( (d_s = 0) \) in a system of 3D spins \( (d = 3) \) on 2D lattice is shown, and the continuous transformation which destroys the defect is easy to construct. The transformation in order parameter space that achieves this is also shown in Figure 12. The existence of such an escape to the free dimension is best visualized in order parameter space. If the dimensionality of the order parameter space is higher than the dimensionality of the defect core, the defect can always be distorted into a continuous region. In Figure 12 a 1-dimensional loop around the equator (representing the core of the defect) of the 3D sphere (representing the order parameter space - note that the sphere in 3D is itself a 2D object) is slid off the sphere and deforms into a point. A similar deformation can be constructed every time the condition \( d' < n \) is satisfied \textsuperscript{2}.

On the other hand, if \( d' > n \), it is impossible to construct a configuration where the order parameter changes continuously around the core. There is not enough dimensions left in order parameter space to make a continuous change. For instance in a 2D Ising model where \( n = 1 \) and \( d = 2 \) it is impossible to create a point defect. If the order parameter changes, this constitutes an discontinuous change resulting in a line defect rather than a point defect.

\textsuperscript{2}The defect that can be removed by a continuous distortion also represents a state with higher free energy density as the state with no defect. Therefore this configuration never appears in real systems \cite{5}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure10.png}
\caption{Formation of boundaries in a transition into a configuration of spins without defect \cite{1}.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure11.png}
\caption{Annihilation of a topologically unstable defect with a continuous deformation in an aligned state. This is possible since \( d' < n \) (\( n = 2 \), \( d = 3 \) and \( d_s = 0 \)) \cite{1}.}
\end{figure}
Figure 12: Continuous distortion of a vortex in \( n = 3 \) parameter space on a plane \( (d = 2) \). The loop can be continuously distorted into a point at the pole [1].

3 Defects in ordered media

Apart from the example already mentioned, there are many interesting defects in other systems as well. Some of these systems are mentioned below.

3.1 3D spins in 3D space

The system of 3D spins in 3D space can form stable point defects \((n = 3, \ d = 3\) and from \(d' = d - d_s = n\) follows \(d_s = n - d = 0\)), some of them are shown in Figure 13. The order parameter space is a sphere \(\mathcal{M} = S_2\) and similarly to the previous example, we can assign integer values of “charge” \(k\) to different defects. The integral definition of charge is

\[
q = \frac{1}{8\pi} \oint_{\sigma} \epsilon_{ijk} \hat{n} \cdot \left( \frac{\partial\hat{n}}{\partial x_j} \times \frac{\partial\hat{n}}{\partial x_k} \right) dS_i
\]  

where \(\epsilon_{ijk}\) is the Levi-Civita totally asymmetric tensor and \(\hat{n}\) is the director field. We integrate over a closed surface \(\sigma\) surrounding the defect core and the value of \(q\) represents the number of times the mapping of the surface enclosing the core wraps the order parameter space \(S_2\). The surface must be defect-free [6]. A charge of +1 can be assigned to defects (a) and (b) in Figure 13 and a charge of −1 can be assigned to defects (c) and (d). By rotating all spins for 180° around \(z\) axis (which is a continuous distortion), configurations in (b) and (d) transform into configurations in (a) and (c) respectively.

Figure 13: Hedgehog defects in 3D space [1].

3.2 Smectic liquid crystals

Smectic liquid crystals are liquid crystals that arrange themselves in layers, and the director (vector that points into the direction of the main axis of liquid crystal molecule) is constant in each layer, but depending on other parameters it may differ between layers, therefore smectic LC need two order parameter fields for characterization: the director field and the layer displacement field. As we are interested in defects in arrangement of layers, we will use the layer displacement field for description of order. Planes are defined by relation

\[
z - u(\vec{r}) = kd = 2k\pi/q_0
\]

where \(d\) is a distance between layers in \(z\) direction (this notation is kept throughout this section) and \(u(\vec{r})\) is a displacement in \(z\) direction and serves as an order parameter in this model. Because of this, the
order parameter space is identical to the direct lattice of smectic planes and thus can be represented by either a unit circle or a real axis with points \( x = 2k\pi \) identified (the same as in the case of 2D spins in 2D space).

To be able to later generalize our findings it is convenient to define Burgers vector \( \vec{b} \) as

\[
\vec{b}(r) = kd\vec{e}_z
\]  

A Burgers vector is a vector that represents the magnitude and direction of the lattice distortion. The set of Burgers vectors is equivalent to the direct lattice. It is used to describe a lattice distortion.

As the parameters of this system are \( n = 2 \) and \( d = 3 \), only line defects are stable \((d_+ = n - d = 1)\). A line defect can be therefore characterized by the relation

\[
\int_{\Gamma} d\vec{u} = \vec{b} = kd\vec{e}_z
\]  

As \( \vec{u} \) and \( \vec{b} \) have a direction, the nature of the defect depends on the direction of the core \( \vec{l} \) relative to \( \vec{b} \). If the core \( \vec{l} \) is parallel to \( \vec{b} \) and \( k = 1 \), then \( \vec{u} \) changes by \(+d\) in one circuit of the core (which passes through the origin in the \( xy \) plane) and the equation determining the position of smectic planes is

\[
z - \frac{d}{2\pi} \Phi(x, y) = kd
\]

\[
\Phi(x, y) = \tan^{-1}\left(\frac{y}{x}\right)
\]  

This means that a plane containing positive \( x \) axis will increase in height for \( d \) (one width of a level) when it encircles the defect at origin once in counterclockwise direction. This is called a screw dislocation and is shown in Figure 14. Winding number \( k = 1 \) means that the planes raise for half of the plane height when rotating for 180°. The plane raises when moving from left to right in front of the core if \( \vec{b} \parallel \vec{l} \) [1].

In the case where \( \vec{l} \) is perpendicular to \( \vec{b} \), edge dislocations are formed. The equation defining smectic planes in this case becomes:

\[
z - \frac{d}{2\pi} \tan^{-1}\left(\frac{z}{y}\right) = kd + u_0
\]  

In this type of defect, for the case where \( \vec{b} = d\vec{e}_z \), one layer is inserted from the left at the defect line. In Figure 15 the layers for the case where \( \vec{b} = \pm a\vec{e}_x \) are shown.

Defects with \( \vec{b} = ad\vec{e}_z + \beta d\vec{e}_x \) are also possible, and are a linear combination of both presented defects.

The lines of defect core must either terminate at the sample boundary, or form closed loops inside the sample. Closed loops lying entirely in \( xy \) plane are pure edge loops and correspond to an additional layer of atoms inside the loop or removal of a layer of atoms from the interior of the loop.

In is also interesting to know, that in the case of smectic liquid crystal, the increase in free energy per unit length of the defect line does not diverge with the size of the sample, as in the case of 2D spins in 2D lattice in equation 11. The increase in free energy per unit length is

\[
F/L = D\frac{d^2}{4\pi} \ln(\lambda_2/a)
\]  

where \( \lambda_2 = \sqrt{K_2/D} \) is the twist penetration length and depends on material dependant constants [1, p.538]. Derivation of this equation is outside of the scope of this seminar.
3.3 Periodic solids

In periodic solids, the order parameter is the atom displacement field vector $\vec{u}(\vec{r})$, and the order parameter space $\mathcal{M}$ is a $n$ dimensional space with lattice points identified. An alternative representation of the order parameter space as a $n$-dimensional torus is also possible (but it might become unintuitive when $n > 2$). The integral definition of the quantity describing the defect is similar to the definition we used for defining the winding number in 3 (the equation 3 can be seen as a special case of this equation, where we took $\theta$ as order parameter)

$$\int d\vec{u} = \int_{\mathcal{M}} \frac{d\vec{u}}{ds} ds = \vec{R} = \vec{b}$$

and defines a Burgers vector $\vec{b}$ of a crystal. In periodic lattice, the Burgers lattice and the direct lattice are equivalent, therefore we can assign a point in direct lattice to every defect in the same way as we assigned a winding number to each vortex in the first example.

Examples of edge dislocation and screw dislocation - the same types of dislocations that appeared in smectic crystals - are shown in Figure 16. A simple method of determining Burgers vector of a known deformation is also shown in Figure 17 and the procedure is as follows: first (a) create a closed path in undistorted crystal (any closed path with steps only between closest neighbours in crystal lattice will do), and then (b) reproduce the steps taken on the path from previous example so that it encloses the core of the defect. The Burgers vector is the vector pointing from the beginning to the end of the new path ($SE$).

We can also visualize a construction of deformation by cutting a cylinder oriented along the $z$ axis along the $yz$ plane. The material on both sides is then displaced by $\vec{b}$ relative to one another and glued together. This process is known as volterra construction. This is only possible when $\vec{b}$ is a vector of the direct lattice, as only in this case the atoms line up correctly. The process is shown in Figure 18 for different Burgers vectors $\vec{b}$. Despite the differences in figures (a) and (b), we can transform one defect into another by a simple rotation of the coordinate system. Both defects represent a defect in which one

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**Figure 15**: Plane displacement (a) and edge dislocations for $\vec{b} = \pm d \hat{e}_z$ (b) and (c) [1].

**Figure 16**: Edge and screw dislocation in solids [1].
extra layer is inserted at the core, in defect (a) the inserted layer is vertical, and in defect (b) the inserted layer of atoms is horizontal. Figure (c) represents a screw dislocation. It is also possible to twist the two sides by an angle before gluing them together. In this way we can construct twist and wedge defects, as shown in Figure 19.

**Figure 17:** Obtaining a Burgers vector \( \vec{b} \) of a dislocation [1].

**Figure 18:** Volterra construction for different Burgers vectors \( \vec{b} \). Figures (a) and (b) represent edge dislocation where an extra layer of atoms is inserted vertically and horizontally respectively, and figure (c) represents a screw dislocation [2].

### 3.3.1 Disclinations in solids: twist and wedge

Another class of defects exists in solids which is similar to the class of defects that appear in smectic liquid crystals and involves distortions in rotational symmetry (the defects already covered involved distortions of translational symmetry). These defects have a high energy barrier and therefore do not appear often in the solid phase.

Their construction can be visualized by the volterra construction (shown in Figure 19). Instead of shifting the lattice before gluing, the lattice is rotated. Depending on the symmetry of the system, only specific angles of rotation are possible (in cubic lattice only rotations by a multiple of 90° are possible). The resulting defects are shown in Figure 20.

### 3.4 Blue phases of liquid crystals

Blue phase of a liquid crystal is a phase in which molecules form structures with long range three dimensional orientational order. These structures have cubic symmetry, so they can be treated as solid crystals with this symmetry, and as such also show similar topological defects as solid crystals. A detailed explanation of how these defect lines form and why they are stable is beyond the scope of this seminar, but we should mention that a winding number of \( k = -1/2 \) can be assigned to these defect lines. We can
**Figure 19:** Constructing twist and wedge dislocations: figures (a) and (b) show twist dislocations and figure (c) represents wedge dislocation [7].

**Figure 20:** Examples of (a) $+90^\circ$ wedge, (b) $-90^\circ$ wedge, (c) $+90^\circ$ twist and (d) $-90^\circ$ twist in a solid with cubic lattice [1].

Think of topological defects in these phases as of topological defects in spatial ordering of the defect lines, which are topological defects by themselves. Figure 21(a) shows how molecules are oriented in a unit cell of blue phase 2 and Figure 21(b) shows defect lines with $k = -1/2$ in this cell. Figure 21(c) shows how defect lines are arranged in blue phase 2 in a region around the core of a screw defect with $k = 1$, and Figure 21(d) shows a screw defect in blue phase 1, as observed in an experiment.

**Figure 21:** Topological defects in blue phases. Figure 21(a) shows orientation of molecules in blue phase 2 [11], Figure 21(b) shows defect lines in one cell of blue phase 2, Figure 21(c) shows defect lines around a core of a screw defect with $k = 1$ (work of the author) and 21(d) shows a screw defect in blue phase 2, as observed in an experiment [12].

## 4 Effects of defects on physical properties of materials

### 4.1 Crystal growth

Crystals grow by attaching atoms to the sides of the crystal seed [1]. As it is energetically less favourable for the atoms to attach to an exposed side than to an inverted edge, crystals with more edges grow faster.
A screw defect, for example, creates such an edge that is continuous in one direction, and therefore aids to the crystal growth (see Figure 22).

**Figure 22:** An exposed edge of a screw dislocation provides a place where the atoms can easily attach and therefore aids to crystal growth [1].

### 4.2 Crystal strength

The *yield stress* $\sigma_m$ of a crystal (the maximum stress to which it can be subjected without breaking) can be determined by estimating how much stress is needed for the atoms to move in the lattice for a half of lattice spacing $(a/2)$; in such a case one can say the lattice has yielded (Figure 23) [1].

We can estimate the stress needed by extrapolating the result for small displacements

$$\sigma \sim \frac{\mu a}{2\pi c} \sin(2\pi x/a) \rightarrow \frac{\mu x}{c} \text{ for } x \rightarrow 0$$

which gives

$$\sigma_m = \frac{\mu a}{2\pi c} \sim \frac{\mu}{10}$$

Estimate can be refined, but it always remains in the same order of magnitude. Measured values for $\sigma_m$ are much lower, in order of magnitude from $\sigma_m = 10^{-4}\mu$ to $\sigma_m = 10^{-2}\mu$. In the case of commonly used standard A36 steel this is $\sigma_m = 250MPa$. This difference can be explained by taking into account the effects of edge dislocation defects. In our estimate we have presupposed a defectless crystal with perfect lattice. In crystals where edge dislocation defects exist, only a single atom at a time (as shown in Figure 24) switches its position and the defect moves through the crystal. On the first figure (a) the inserted edge is $AA'$. When stress is applied, the atom $E$ moves to the other side of the inserted plane, and the defect moves so that on figure (b) the edge $BB'$ represents the inserted edge. This process is called *glide* and the plane in which it appears the *slip plane* and greatly reduces the strength of the crystal.

To avoid this, the defects can be pinned to impurities so they cannot move freely. This is process is called work hardening.

**Figure 24:** Propagation of an edge dislocation through a crystal [1].
5 Conclusions

Topological defects affect order in crystals and other ordered media in sometimes quite unexpected ways. The formal description provided by topological invariants has given us a useful way of categorizing the defects and separating them into classes. Topological defects of different origin and characteristics are introduced, including vortices in 2D spin systems, hedgehog defects in 3D spin systems, plane dislocations and screw defects in crystals, and twist and wedge defects in solid crystals. As we encounter new phenomena, it is often necessary to adopt new mathematical tools that aid us to understand new phenomena. The theory and language of algebraic topology had proven useful in the study of topological defects. It also gives some nontrivial insights into what we can observe, and in this seminar a few examples of what it has to offer were given.

As topological crystals prove crucial in understanding crystal growth and strength, it is important to understand the related phenomena when very precise material properties are wanted. For instance, monocrystalline silicon is of great importance in semiconductors (perfect crystals of silicon are needed to build integrated circuits and processors). Topological defects also play a crucial role in understanding the behavior of nematic colloids which because of interesting optical properties are of great research interest [3]. Besides applications in soft and solid matter physics, these defects are also important in cosmology: hypothetical cosmic strings are topological defects of the space itself [8].

References