Defects in Crystals

Faizan Nazar
MASDOC, Mathematics Institute, University of Warwick

Introduction

When it comes to building electrical devices, nowadays manufacturers want to build devices that are as small as possible. However, they are approaching a fundamental limit as they are reaching the scale of building objects out of individual atoms.

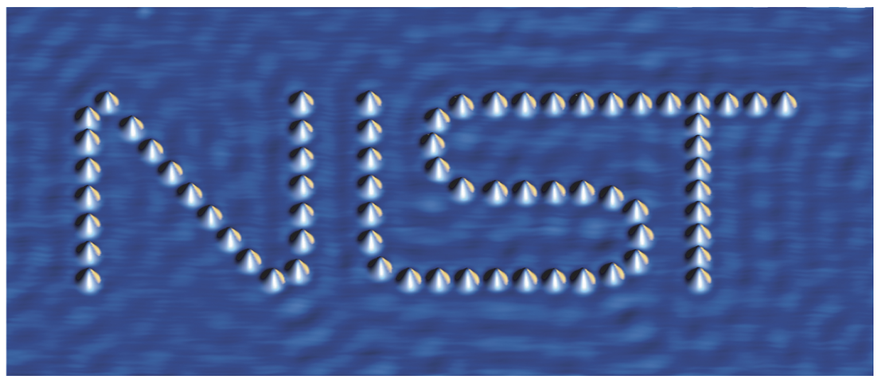

Figure : Image by Joseph Stroscio, Robert Celotta (NIST). In 2004, physicists at the National Institute of Standards and Technology (NIST) in the US spelt out the company logo by arranging individual atoms, by hand! This work was pioneered by researchers at IBM and in 2013, they used this idea to make a stop-motion video called 'A Boy and His Atom' - look it up on youtube.

This image from the NIST was made by arranging cobalt atoms over a copper background, using a scanning tunnelling microscope. The picture allows us to see each atom separately, even though they were just a few nanometres apart.

Copper is a highly conductive material, as the copper nuclei are surrounded by a sea of free electrons. These electrons can move through the material and transfer an electric charge with them, conducting electricity. Adding cobalt atoms to the copper will introduce more nuclei and electrons, which will effect the conductivity of the material.

Doping

Circuits are built from silicon these days (though researchers are also into looking into new materials like graphene), but manufacturers also introduce different atoms into a material, to change how it conducts electricity. This process is called doping.

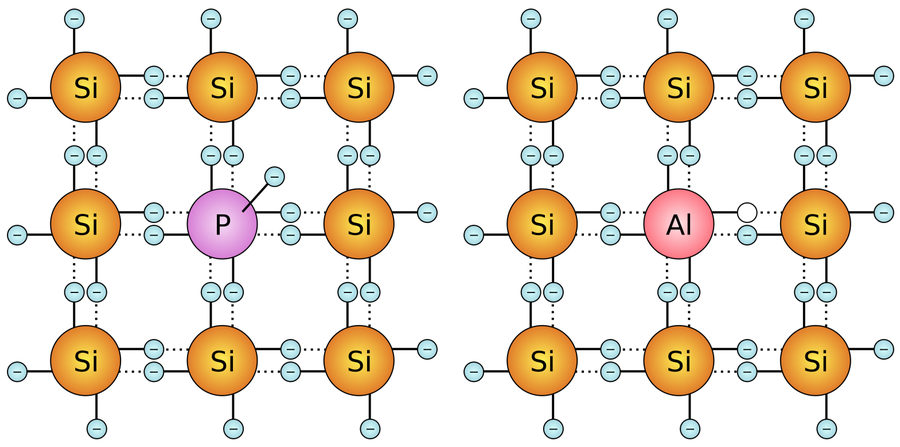

Figure : n-type (Phosphorus) and p-type (Aluminium) doping of silicon. Images by Wikipedia user Cepheiden.

The new material is called a semiconductor. There are two types of doping, called p-type and n-type, short for positive and negative, respectively. Each types of doping changes how charges are carried through the material.

Both p-type and n-type doping are used together to make transistors, which are the building blocks for all electrical devices. These days a single computer can contain billions of transistors.

My research

The aim of my research is to understand the effects of introducing a local defect in a crystal (a material with a regular order). A local defect could represent an impurity, interstitial or vacancy.

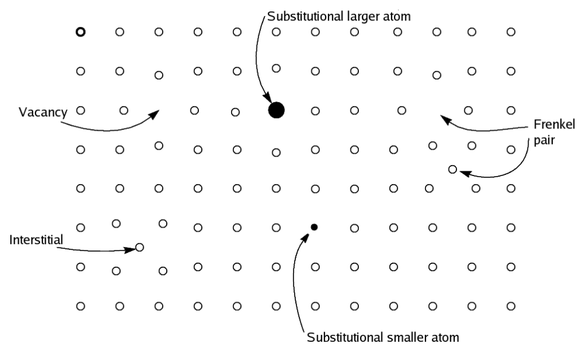

Figure : Examples of local defects in a crystal. Image by Kai Nordlund.

In particular, I am interested in the re-arrangement of the crystal structure that would occur due to the presence of a defect. For example, if the defect has a strong positive charge, one might expect that it would cause a repulsion of the surrounding nuclei. I am interested in finding out if the introduction of a defect effects the entire crystal, or only the nuclei that are close to the defect.

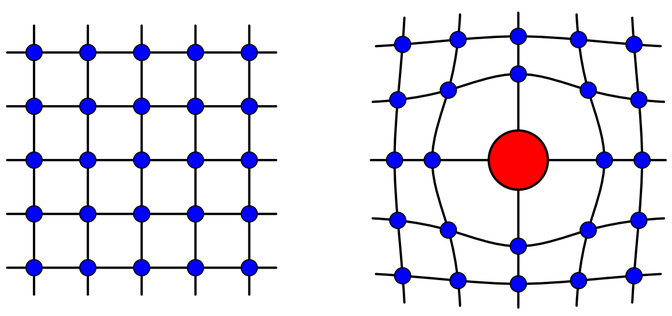

Figure : A 2D sketch of a perfect lattice and a lattice which has been re-arranged due to the presence of a local defect.

To do this, we consider the possible re-arrangements that could occur, then aim to find the re-arrangement that minimises the energy of the system. We use the Thomas-Fermi-von Weiszacker model, which gives a simplified quantum description of the crystal.

Once we have found a lattice displacement that minimises the energy of the system, we wish to understand it's properties. For example, we would expect that eventually the displacement becomes smaller further away from the defect. We wish to describe this effect mathematically, by showing decay properties for a minimising displacement.

The Model

To describe the system, we use $u, \phi, m : \mathbb{R}^3 \to \mathbb{R}$, where

- u - the root electron density, $u \geq 0$.
- m - the nuclear distribution, $m \geq 0$.
- ϕ - the Coulomb potential generated by u and m.

Using these, the Thomas-Fermi-von Weiszäcker energy of the system is defined by

$$E^{TFW}(u, \phi, m) = \int_{\mathbb{R}^3} |\nabla u|^2 + \int_{\mathbb{R}^3} u^{10/3} + \frac{1}{2} \int_{\mathbb{R}^3} \phi(m - u^2).$$

The first two terms describe the kinetic energy and the last term describes the Coulomb energy of the system due to the charged particles. Given a nuclear distribution m, minimising the energy per unit volume gives a ground-state (u, ϕ), which solves

$$-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0,$$
$$-\Delta \phi = 4\pi(m - u^2).$$

The existence and uniqueness of a solution to this system is guaranteed under broad assumptions on m.

A local defect is described by $\rho^{nuc}_{def} \in C^\infty_c(\mathbb{R}^3)$, and we consider the space of lattice displacements

$$\mathcal{W}^{1,2}(\Lambda) = \left\{ U_\Lambda : \Lambda \to \mathbb{R}^3 \;\middle|\; \left(\sum_{l \in \Lambda} \sum_{i=1}^{3} \frac{|U_\Lambda(l + a_i) - U_\Lambda(l)|^2}{|a_i|^2} \right) < \infty, \lim_{|l| \to \infty} U_\Lambda(l) = 0 \right\}.$$

Let $U_\Lambda \in \mathcal{W}^{1,2}(\Lambda)$ lattice displacement and let $\eta \in C^\infty_c(\mathbb{R}^3)$ be a positive function describing an individual nucleus, then we are interested in the following nuclear distribution

$$m_{U,def}(x) = \sum_{l \in \Lambda} \eta(x - l - U_\Lambda(l)) + \rho^{nuc}_{def}(x)$$

and it's corresponding ground-state $(u_{U,def}, \phi_{U,def})$. Similarly we can define m_U and (u_U, ϕ_U), which describes the system where the displacement U_Λ rearranges the nuclei, but no defect is present.

The Energy Difference

Using the ground-states (u_U, ϕ_U), $(u_{U,def}, \phi_{U,def})$, consider the two energy differences

$$\mathcal{E}(U_\Lambda) = E^{TFW}(u_U, \phi_U; m_U) - E^{TFW}(u_{per}, \phi_{per}; m_{per}),$$
$$\mathcal{E}^{def}(U_\Lambda) = E^{TFW}(u_{U,def}, \phi_{U,def}; m_{U,def}) - E^{TFW}(u_{per}, \phi_{per}; m_{per}).$$

Provided $\mathcal{E}^{def}(U_\Lambda)$ is well-defined for each $U_\Lambda \in \mathcal{W}^{1,2}(\Lambda)$, define

$$\mathcal{I}^{def} = \inf\{ \mathcal{E}^{def}(U_\Lambda) \,|\, U_\Lambda \in \mathcal{W}^{1,2}(\Lambda) \}.$$

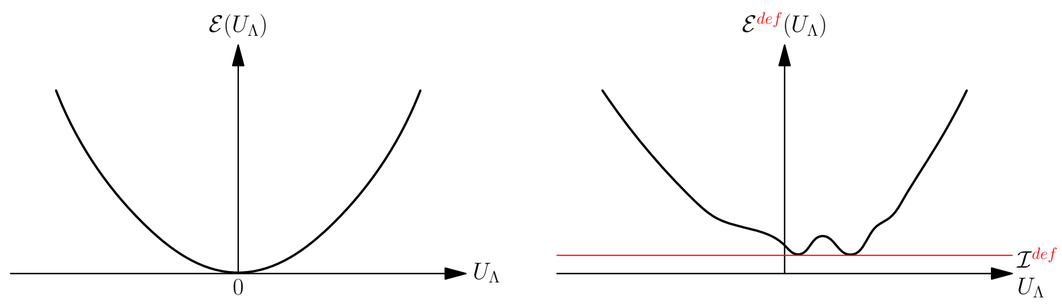

Figure : A sketch of the energy difference without a defect, and the difference with a defect.

The main tool for studying both energy minimisation problems is the following result.

Exponentially-weighted Estimates

Suppose $R_1, R_2 \in C^k(\mathbb{R}^3) \cap W^{k,\infty}(\mathbb{R}^3)$ *for some* $k \in \mathbb{N}$. *Suppose further that* $\inf u_1 > 0, \inf u_2 > 0$, $u_1, u_2, \phi_1, \phi_2 \in C^{k+2}(\mathbb{R}^3) \cap W^{k+2,\infty}(\mathbb{R}^3)$ *and that* $(u_1 - u_2, \phi_1 - \phi_2)$ *solve the following system*

$$-\Delta(u_1 - u_2) = \frac{5}{3}\left(u_2^{7/3} - u_1^{7/3}\right) + \phi_1 u_1 - \phi_2 u_2 + R_1,$$
$$-\Delta(\phi_1 - \phi_2) = 4\pi\left(u_2^2 - u_1^2\right) + R_2.$$

Then there exists $C_k, \widetilde{\gamma}_k > 0$ *such that for all* $0 \leq \gamma \leq \widetilde{\gamma}_k$ *and* $\widetilde{x} \in \mathbb{R}^3$

$$\sum_{|\alpha| \leq k+2} \int_{\mathbb{R}^3} \left(|\partial^\alpha (u_1 - u_2)(x)|^2 + |\partial^\alpha (\phi_1 - \phi_2)(x)|^2 \right) e^{-2\gamma|x - \widetilde{x}|} dx$$
$$\leq C_k \sum_{|\beta| \leq k} \int_{\mathbb{R}^3} \left(|\partial^\beta R_1(x)|^2 + |\partial^\beta R_2(x)|^2 \right) e^{-2\gamma|x - \widetilde{x}|} dx.$$

If in addition, $G_1, G_2 \in H^k(\mathbb{R}^3)$, *choosing* $\gamma = 0$ *gives*

$$\|u_1 - u_2\|_{H^{k+2}(\mathbb{R}^3)} + \|\phi_1 - \phi_2\|_{H^{k+2}(\mathbb{R}^3)} \leq C'_k \left(\|G_1\|_{H^k(\mathbb{R}^3)} + \|G_2\|_{H^k(\mathbb{R}^3)} \right).$$

In short, a small perturbation of m ***causes an exponentially decaying response in*** u, ϕ***.***

Applications

This exponential estimate is vital in investigating the properties of $\mathcal{E}^{def}$, such as its regularity as a functional. With Taylor's theorem in mind, we can express $\mathcal{E}^{def}$ in terms of it's derivatives, so for $U_\Lambda \in \mathcal{W}^{1,2}(\Lambda)$ we have

$$\mathcal{E}^{def}(U_\Lambda) = \langle \delta\mathcal{E}^{def}(0), U_\Lambda \rangle + \int_0^1 (1 - t) \langle \delta^2 \mathcal{E}^{def}(tU_\Lambda) U_\Lambda, U_\Lambda \rangle \, dt.$$

We can study $\mathcal{E}^{def}$ by investigating the right-hand side of the above equation.

Conclusion

Using the results that we have shown, we aim to show that the energy minimisation problem with a defect is well-defined. Further to this, we wish to understand the decay properties of a minimising displacement.

Acknowledgements

This poster is based on joint work with Prof. Christoph Ortner.

EPSRC Pioneering research and skills