# 6. The Iron-Carbon Phase Diagram

## 6.1 A Map for Steel

### 6.1.1 It Takes Two to Tango

**Famous First Words**

- Perfect crystals are boring. They have the properties they have, and you can take it or leave it, but you cannot change them without destroying perfection. What we want in a first step now are *almost* perfect crystals that contain some defects.
  - Even **diamonds** (relatively perfect carbon single crystals) are more valuable if they contain a few defects that give them some color. A perfect aluminum oxide ($Al_2O_3$) crystal is not even seen as a gemstone. Contaminate it with a tiny bit of chromium or titanium, and now it's a **ruby** or a **sapphire**, respectively.
    Gemstones are quite useful for obtaining favors from desirable ladies, so I give you a special module that might help you to score without having to actually buy one of those expensive baubles.
    You might, for example, expostulate about the fact that the first **Laser** was made from a (synthetic) ruby, and that the decisive thing for getting rubies to be red is to have a few chromium atoms in there, dissolved as substitutional point defects in an otherwise boring aluminum oxide crystal.

    You should be able to score without actually having to buy a ruby, in particular if the female in question is of the **Angela Merkel** type 1).

    **Advanced Link**

    **Gemstones**
  - If I'm right and perfect crystals are boring, you might wonder why we are going through great pains to make silicon crystals as perfect as possible? It's for the same reasons why some time ago my forebears, and possibly yours too, wanted their women to be "perfect", i.e. virgins: you want to destroy the perfection in a *controlled* way. As far as silicon is concerned, doping it with suitable **impurity atoms** in precise amounts doesn't make much sense if all kinds of other unknown defects have already left their traces in there.
- It needs two to tango, and if we want things to get a bit more interesting, we must bring our prissy perfect crystal into intimate contact with atoms of a different kind.
  - Making swords or any other *steel* objects in antiquity meant to put at least one other kind of atom into the rather pure iron. Typically this was carbon but there was also a lot of **phosphorous (P) steel**. It matters very much exactly how much carbon (or phosphorus) atoms are put into the iron crystal, and what they are doing in there.
    It also matters very much what *else* is in there in terms of defects.
- I'm talking about the *core process* for much of materials engineering. The best example besides iron and steel technology is **semiconductor technology**. It's all about **defect engineering**.
  - If we make **microchips** from perfect silicon crystals, we put a precisely defined number of phosphorous (P), Arsenic (As) or boron (B) atoms in precisely defined tiny volumes (about 0,1 $\mu m^2$ square and 0.01 µm deep). More, we need to make sure that the crystal accepts and keeps them there as substitutional impurity atoms. We also want to be sure that there are no other defects present.
  - Things are far more relaxed with iron and carbon. Nevertheless, when we put carbon atoms inside iron crystals, the kind of their arrangement is important for what we have in mind .
- Crystals, however, have a mind of their own and usually don't like what we do to them. They will fight back. They always stick to the second law in letter and spirit as much as they can, and they don't care about your desires. It's like having a virgin who wants to be a nun.
  - Whenever you put foreign atoms inside some crystals in some particular way, it might not be the way they want things to be. Then they will do their best to rearrange everything in such a way that they get as close as possible to nirvana once more. All they need is some temperature and some time to move atoms around, and you should be quite aware of that.
- The first order of business now is to find out what a crystal, if left to its own devices, will do with those foreign atoms you doped, contaminated or *alloyed* it with
  - So ask yourself: If the foreign atoms cannot be gotten rid of, what would a nirvana-seeking crystal do with them? Well, we have dealt with that already. In an *ideal* world or crystal, surplus extrinsic point defects precipitate or are stuffed into grain boundaries. How about in *reality*? Reality meaning that we now look at some defined material **A** that contains a defined and possibly *large* amount of a material **B** at a defined temperature ***T***.
    In other words, we are now looking at the whole range of compositions: from pure **A** via alloys or chemical compounds of **A** and **B** all the way to pure **B**.

What are we going to find for, say, 86,5 % **B** alloyed with 13,5 % **A** at 675 $^{0}$C or 395 $^{0}$C? **A** and **B** could be iron (Fe), carbon (C), nickel (Ni), gold (Au) copper (Cu), molybdenum (Mo) silicon (Si), ..., everything from the periodic table.
With about 90 elements in the periodic table, we have 90 × 90=8100 basic possibilities and for each of these possibilities the whole concentration range. There is a lot of work ahead!

- Never fear. Material scientists and engineers have already done the work. They came up with an ingenious way to illustrate what happens in all these cases (and more):

**They invented phase diagrams**

Phase diagrams are for second-year students of materials science what garlic is for vampires: they scream and run for cover when we whip one out during a lecture course.

- *They* have good reasons for being scared by phase diagrams but that need not concern *you*, the reader.
  Have you ever looked at a **map** before you go places? I bet you did. On your map you saw major and minor streets, forests, cities and towns, railroads, rivers, lakes and oceans. The map even told you how to get to your destination, including possible alternative routes.
- What an outrageous lie! You certainly did *not* see roads etc. on the map! All you saw were lines of various colors and styles, shaded and colored areas, and so on, printed on a piece of paper.

"Seeing" roads and rivers and finding your way resulted from your **interpretation of map symbols**, based on some simple rules that about half of humankind figured out early in life.

- First you find your present location on a map, which in case of doubt is given by two numbers: the vertical (north-south by convention) and horizontal (west - east) distance from some zero point. You also may call these numbers latitude and longitude if you get your scales right.
  Then you figure out how to get from where you are to where you want to go. The map also tells you what you will encounter on your chosen path. Maybe there is a river to cross, you will ride through a forest, or you encounter some towns on the way. It's all there. All you need to know is how to interpret the symbols on the map.

Phase diagrams are pretty much the same thing. They provide a kind of **map** that tells you what you will find in a certain location in the world of materials (mostly crystals) that are made from two kinds of atoms, **A** and **B**.
There is a big difference to geographical maps, however. Phase diagrams *only* show the *ideal state of crystals*, not necessarily the *structure* as you will find it. In other words:

**Phase diagrams show only the "nirvana" state.**

- A good geographic map shows slums, for example, which in an ideal world would not exist. A phase diagram, in contrast, does not show structural "slums", e.g. crystal structures that the crystal hates and would never assume on its own. That doesn't mean that those structures do not exist.

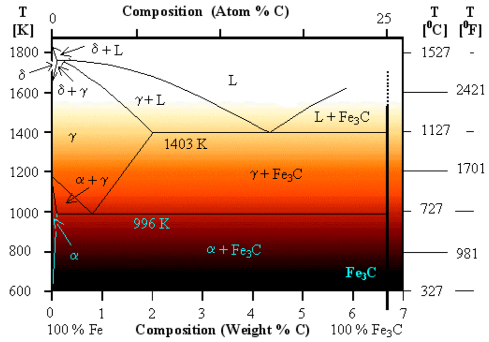
As in a geographic map, two numbers give the starting "location" in a phase diagram. Instead of latitude and longitude we have something different.

1. The *first* number gives the **composition**, the ratio of **A** : **B**. An example for a composition is the percentage of carbon in iron. 1 wt% carbon in iron is a certain composition, and so is 10 wt% tin (Sn) in cupper (Cu). These composition actually have names: steel or bronze, respectively, but most compositions don't.
2. The *second* number gives the *temperature* ***T*** in some scale.

Both numbers are variables that could have any values. Well, not really. Temperatures below the absolute zero point do not exist and temperatures above the melting point are irrelevant in most cases. You also cannot go below 0 % or above 100 % for concentrations, but these limits are rather trivial.

- Easy enough. So why do our students run for cover when we get to phase diagrams? Because we don't just expect that they can "read" a phase diagram, we expect that they can *make* one.
  You can read a map? Cool—but can you make one?
  *Making* a map of Istanbul is a lot of work and needs a lot of skill. In comparison, reading it is laughably *easy*. I won't try to teach you how to make a phase diagram but I teach you how to read one. Only simple ones, of course. This will be sufficient to find out what you can *do* with a phase diagram.

Enough small talk. Let's jump into the cold water (or rather a **heat of steel)**) and look at the **phase diagram** of the *binary* **iron-carbon system**. Here it is:



**The iron - carbon phase diagram**
The colors are usually not there. They only serve to give you, the smith, an idea what the work piece looks like at the temperature indicated.

  - I used big words above but they are rather self-explaining, I hope. "*Binary* " is Latin for "twofold" and thus means that the system we consider consists of a mix of just *two* different atoms. With about 90 different elements, we have 90 · 90=8.100 different binary *systems* we can play with. The **system** iron - carbon is just *one* oft these.

## The Basics About Phase Diagrams

- Now come back - don't run away. It's not as bad as it looks. Let's go over it bit by bit.

  - *First* we note what is depicted.
    From left to right we simply have the **concentration** of carbon in iron. At the bottom it is given in **weight percent** (wt %), at the top, out of the goodness of my heart, I give it in **atom percent** (at %) too.
    We only go up to 7 wt % carbon because nothing of interest to sword making happens beyond this carbon concentration.

    *Second*, from bottom to top we have the **temperature**. On the left it is given in the absolute temperature scale (Kelvin; K), on the right, out of the goodness of my heart, I'm doing a very unscientific thing and give you the Celsius (degree Celsius; $^0$C) *and* the Fahrenheit (degree Fahrenheit; $^0$F), scale, too.
    I have omitted temperatures below 600 K (327 $^0$C, 621 $^0$F)) because nothing of interest happens there as far as the *phase diagram* is concerned.
    As far as *sword making* is concerned, interesting things may still happen below that temperature; I'll come to that

  - The Greek letters α, γ, and δ, the "L", and the chemical shorthand $Fe_3C$ in the phase diagram simply refer to the *different* phases one encounters in the iron - carbon system.
    The background color is a feeble attempt to reproduce the color that hot iron shows when it glows. It's red-hot around 1100 K (827 $^0$C, 1520 $^0$F) and bright yellow around 1350 K (1077 $^0$C, 1971 $^0$F).

- By the way, the color of a hot body does not depend very much on what that body is composed off. If we would heat you, dear reader, to a temperature of 1400 K (1127 $^0$C, 2061 $^0$F), you would glow bright yellow, just the same as iron or anything else. OK - I agree that you might sizzle a bit, giving off various aromas during the process of heating. But that is not important. Whatever is left will be glowing bright yellow.

  - It was **Max Planck**, who first came up with an explanation for this strange fact in 1900 (in terms of a precise mathematical equation), opening the gate to quantum theory and thus to Materials Science.

- Now you have seen one phase diagram—for iron-carbon—but there are many more. If you think about it once more for a second, you realize that for all materials consisting of just *two* kinds of atoms, about 90 × 90=8.100 phase diagrams exist, since we have about 90 different kinds of atoms.

  - We actually know most of those **binary phase diagrams**, thanks to all these students spending a lot of time constructing them. Coming up with a new phase diagram is a typical PhD thesis; it does take a lot of brain and effort.

  - We can, of course, come up with roughly 90 × 90 × 90=72.900 *tertiary* or three-fold phase diagrams for materials with *three* different kinds of atoms (kind of hard to draw). Iron with some carbon *and* some manganese (Mn) would be a relevant example.
    We have about 65.610.000 *quaternary* phase diagrams for materials with *four* kinds of atoms (impossible to draw but possible to express in formulas), and so on.

- Our common "alloy steels" of today comprise *at least* four kinds of atoms, usually more. You would run for cover, too, if you suspect that you would be called upon to construct one of those.

  - Relax. The good news is that after materials scientists mastered the art of turning silicon crystals into microprocessors and the like, we now command tremendous computer power and we are increasingly *calculating* phase diagrams with little effort.
    All you need is the second law and some good idea of how different kinds of atoms relate to each other (and, of course, about 5 - 6 year of your time to learn how it's done).

- If we just limit ourselves to the most simple *binary systems* (two kinds of atoms), the essential input into our phase diagram calculations is how those atoms relate to their own kind *and* to the other one.
  Do they only love each other ("I don't want to be close to this stranger; I want to be with you"), do they like the other kind ("so he is a foreigner, but I just love him more than you"), or do they not give a damn ("I don't care about you or anybody else")? If you could deal with your teenagers, you shouldn't have much of a problem with this.
  If we know these relations, we can calculate precisely what the atoms of a crystal are going to do. Even so the single atoms may do their thing at random, we can predict with certainty what they will do as a group. Teenagers, while being chaotic individually, are also quite predictable as a group.

So gird your loins and follow me. We will now plunge into the intricacies of the iron-carbon phase diagram and find out how it relates to sword making.

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1) Dr. Angela Merkel, the present chancellor (or is to chanceleress?) of Germany and thus the most powerful lady on this planet, is a physicist by training. She is (happily!) married to Professor Sauer, a quantum chemist, who is actively working and well known in his field. He would never even dream of playing "first husband".