**Steel Chemistry/Substrate White Paper**

The purpose of this white paper is to introduce the reader to the chemical and atomic composition of steel, and how composition affects the choice of base substrates when coating and annealing, depending on the desired final product. The first section of this paper takes the form of a long article, broken down into segments by topic. This is followed by a list of important experiments done at Arcanum and a corresponding summary.

**[Phases]**

In solid metals, atoms are arranged in ordered patterns that form crystalline structures called crystal lattices. The crystal lattice shape is the arrangement of atoms that takes the least amount of energy to maintain. There are several types of patterns these crystal lattices can take, but for what we do, the most important are FCC and BCC lattices. Face-centered-cubic (FCC) crystal lattices have the atoms ordered such that if you were to take a 3 dimensional cut-out of the lattice, you would get a cube with an eighth of an atom at each corner of the cube, and half an atom on each face (hence the name) . The body-centered-cubic (BCC) crystal lattice has the atoms ordered such that, again, if you were to cut a cube out of the many layers of ordered atoms, the cube would have an eighth of an atom at each corner, but instead of half an atom at the face, there would be a whole atom in the center, or body. This is illustrated below[1](https://depts.washington.edu/matseed/mse_resources/Webpage/Metals/metalstructure.htm).

A picture containing game, basketball

Description automatically generated

Crystal lattice structures are important in our work because iron can have different structures at certain temperatures, each with unique properties; most important in our case is that FCC allows for better diffusion than BCC. At room temperature, iron has a BCC structure; this is called the ferrite phase, also known as the alpha phase. As temperature increases, it transitions to the austenite (or gamma) phase, which has a FCC structure. BCC is thermodynamically more stable than FCC at room temperature. As temperature increases, both structures increase in energy, but they do so at different rates—BCC increases faster than FCC. At the temperature where the phase transition is, BCC and FCC have the same energy. Any further increase will thermodynamically favor FCC, and cause FCC crystals to nucleate inside the existing BCC structures.

Cr, Al, and Si are ferrite stabilizers, meaning if they are added to iron, it stays in the ferrite phase until a higher temperature. Mn is an austenite stabilizer, so if added, iron becomes austenite at a lower temperature. Cr diffuses better in ferrite than austenite, because FCC structures are less densely packed, since there isn’t an atom in their center. These three facts make up the Arcanum process.

A piece of steel with Cr near the surface and Mn inside (i.e. in the bulk), heated up to a diffusion temperature, will be ferrite at the surface, because Cr stabilizes the ferrite phase, and austenite in the bulk, because Mn stabilizes the austenite phase. Since Cr has different diffusion rates for the two phases, Cr will diffuse through the ferritic surface, but not through the austenitic bulk, resulting in a very defined alloy “layer”. This has a practical benefit in that Cr is concentrated at the surface, to enhance corrosion performance, whereas it would be wasted in the bulk and additionally this allows the bulk of the steel to maintain important mechanical properties, such as formability.

For each element, and each group of elements, the phases and the temperatures at which the phases change can be mapped out. These maps are called phase diagrams. An example of the FeSi phase diagram is shown below, made using OpenCalphad, a free phase diagram software.

A close up of a map

Description automatically generatedThe y axis shows the temperature in Kelvin at which phase transitions occur, and the x axis shows the percent of Si in the FeSi compound, from 0 to 100%. As mentioned before with the ferrite stabilizers, the presence of additional elements (in this case Si), and the amount of said element present, can affect the phases and transition temperatures.

**[Grains]**

A grain is a region in the iron/steel where all the crystal lattices have a specific ordered orientation, although each region will not have the same orientation as its neighbors. When all crystal lattices in an area have the same orientation, they appear as a crystal, or grain. Grain boundaries are the places where grains, or regions with different orientations, intersect. Two adjacent grains cannot have the same orientation, because if they did, there would be no boundary and they would actually be one larger grain.

At high temperatures, small grains dissolve and regrow as a part of a larger grain. This is called Ostwald Ripening. When hot metal cools, small crystals (grains) begin forming and growing as new grains. The longer the cooling process takes, the more time the crystals have to grow, leading to larger grains. This can be thought of as the ordered atoms becoming less ordered (instead of a rigid structure in a solid, a molten/liquid metal would have relatively “looser” structures, or atoms with more movement) as the metal heats up, and then reforming the ordered crystal lattice structures when cooling back down.

Smaller, finer grain sizes improve the strength of a material. When a material is deformed, the grains move within. In order for the grains to move, they must move along the borders (grain boundaries) of other grains. Moving along these boundaries takes energy, so the finer the grains, the more grain boundaries, the more energy it takes to deform the material. Finer grains also increase a material’s ability to deform without failing (breaking). This is because with a high number of grains, it is more probable that when an outside force is applied, it is applied along a number of grain’s slip plane (i.e. instead of having to push/move the grain, it slides/slips). Electrical Steels typically have large, wide, grains, but since they are stamped, they do not need the formability that other steel does.

The standard we use for determining grain size is the ASTM grain size number. The formula is

G = (N+1)/2 where N is the # of grains per square inch at 100x magnification and G is the grain size number. Note that since the formula is based on the number of grains rather than the size of a grain, a higher ASTM equals a smaller, more fine grain. Arcanum aims for ASTM 7 or ~40 microns, although up to ASTM 5 is sometimes considered acceptable, depending on the material.

Exerting force on a metal, such as rolling it or otherwise causing it to plastically deform, can cause its grains to deform from the mechanical stress. These deformed grains are undesirable since their defects can weaken the metal, reducing ductility and elongation. It is possible to replace the undesirable deformed grains with new, no-defect grains through a process known as recrystallization. As discussed above, as a metal heats up and cools down, grains form. Deformed grains store energy when they are deformed, and in conjunction with the annealing process, this energy is used to cause new grains to nucleate and grow from the grain boundaries, “consuming” the deformed grain.

The temperature at which recrystallization starts depends on several factors. As a grain becomes deformed, it stores some of the energy used to deform it. A more deformed grain would therefore have more energy, so new grains nucleate easier – this decreases the recrystallization temperature. Since grains tend to nucleate from grain boundaries, finer grains typically have reduced recrystallization temperatures, since they have more grain boundaries. Reducing the recrystallization temperature can be helpful for getting desirable mechanical properties, since as it decreases, the rate of grain nucleation will increase faster than the rate of grain growth, leading to more fine grains.

A typical use of recrystallization is to heat and then very rapidly cool the metal, so that grains are formed but remain small. Unfortunately, in the Arcanum process, the metal cools relatively slowly since it cannot be quenched, so grain growth can happen.

Along with recrystallization, deformed or stressed grains can also undergo a process known as grain relaxation, or grain recovery. The plastic deformation on the grains manifests as dislocations in the crystal lattice. These dislocations are misaligned atoms in the crystal lattice structure. While recrystallization requires a high temperature, or in other words must be thermally activated, grain recovery can happen at colder (but still hot and significantly above room temperature) temperatures. When metals are heated at low temperatures, but below the recrystallization point, the energy is used to adjust and rearrange crystal lattices such that a given area has a lower dislocation density, which reduces the stress in the material.

A close up of a map

Description automatically generatedThe “cycle” that grains go through can be thought of as recovery -> recrystallization -> grain growth. Metal is stressed from cold-rolling, and its grains plastically deform. As the metal is heated after this, the grains recover/relax, getting rid of some of the defects, then new grains start forming during recrystallization, and finally these new grains grow, consuming some of the smaller, original “defect” grains. See the image to the left[2](https://www.thefabricator.com/thefabricator/article/bending/grain-size-part-ii-how-metal-grain-size-affects-a-bending-operation#gallery-3).

**[Grain-Pinning Particles]**

One method to maintain fine grains is to use grain-pinning particles. Fine particles in a metal formulation can sit along grain boundaries and exert a “pinning” force. Grain boundaries with these particles in them must create new boundaries around the particles, which is not a favorable energy reaction (in other words, it won’t happen often). Having grain-pinning particles will therefore prevent grains from growing or coalescing together, which leads to fine grains. Particle size and number both affect the amount of total pinning, but generally speaking, many small particles pin more than fewer larger particles. Examples of particles than can pin are AlN, NbN, NbC, TiN, TiC.

IF stands for interstitial free steel, which is steel without interstitial atoms (aka trace/”garbage” elements) sitting inside the BCC Ferrite crystal lattice. In this case, interstitial refers to the ability to sit inside/between the atoms in a crystal lattice structure, i.e. sit interstitially. Refer to the image on the first page; there is space for smaller atoms among the crystal lattice atoms. IF steels still contain C and N, but most of it is usually tied up with Nb and/or Ti so it does not precipitate in the steel. IF steels are desirable because they are more ductile due to not having interstitial atoms.

At the temperatures and times we anneal at, traditional IF steels do not retain their fine grains (see recrystallization). Additionally, traditional IF steels do not have grain-pinning particles at temperature.

**[Grain Pinning Particles & Carbide/Nitride Species]**

Titanium can serve a dual purpose in tying up free carbon so that it cannot form chrome carbide later on and in forming a grain pinning particle. Ideally, a substrate useful to Arcanum would be non-IF steel with 2.2% Ti (enough to tie up all C and provide grain-pinning particles), but steel mills cannot produce that much Ti in their steel. An alternative option is to use Ti and N to form TiN, but this has a notable drawback in that TiN forms before steel does, and creates a relatively small number of large particles, which is less effective. It also leaves behind excess N, as well as excess C because there is no Ti to bind it. Nb can be added, since it precipitates at lower temperatures and can pull out the excess N and C. The standard substrate that Arcanum uses, MXC 25 made by Stelco, takes into account the above. It has grain-pinning particles from TiN, and very little free C, N, or S due to the large Nb added in.

A screenshot of a cell phone

Description automatically generated**[Grades of Steel]**

Carbon steel can be divided into three groups, based on carbon amount: low carbon/mild steels (< 0.3% C), medium carbon steels (0.3 – 0.6 % carbon), and high carbon steels (> 0.6% C).

SAE steel numbering system is one (of many) standards of steel used. Carbon and alloy steels are designated by a 4-digit number. The first is the main alloy element (there is a table that says what each element is), second is top grade, and the last two indicate percent carbon in hundredths. So, for example, a 1060 steel is plain carbon steel with .60 wt% C. 2060 would be the same but Nickel steel.

CRML steel is “cold rolled motor lamination” steel. It is steel designed for use in electrical applications. It has a different chemical composition, such as more silicon, and its core is made from several thin strips (AKA laminations) to reduce eddy current losses[3](https://www.ussteel.com/products-solutions/products/cold-rolled-motor-lamination-sheet).

Another common naming system used is ASTM International standards. These are two numerous to name but can be found easily online.