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Computational metallurgy and changes of scale / Métallurgie numérique et changements d'échelle

Foreword: Numerical metallurgy and scale transitions

Physical metallurgy, the mother of materials science [1], is a sort of "intermediate discipline"; relying on concepts elaborated in physics, in mechanics, and in chemistry, it provides also a bridge between fundamental sciences and engineering sciences, between knowledge valued for itself, and knowledge valued as a tool to elaborate devices. As such, physical metallurgy both provides a scientific approach to alloys and process development, but also gets inspiration from practical questions to nurture a fundamental understanding of the thermodynamics, the transport, and the properties of condensed matter.

As any science, metallurgy starts from a classification process, a taxonomy; by nature, this activity provides a simplified view of reality: for instance phase transformations in the solid state are either diffusive (involving random motion of atoms on distances much larger than interatomic spacings) or displacive (involving a collective and very local shift in their position), mechanical behaviour is ductile or brittle depending whether or not plasticity sets in before fracture.

However, although a house is built with stones like a science is made of facts, a collection of facts is no more a science than a pile of stones is a building (a statement attributed to Henri Poincaré). The classification stage is then followed by a modelling exercise. Metallurgy took a long time to reach this stage where modelling became able first to rationalize the observed behaviours, and now, in very specific cases, to be predictive. The reason for this delay (as a scientific activity, metallurgy is almost as old as astronomy) lies in the complexity of the object. Most of the situations investigated by metallurgists are far from thermodynamic equilibrium. In phase transformation, this is the very condition to obtain the small scale structures interesting for the properties. Understanding plastic deformation, one of the properties of interest for metals and alloys, is even worse: the most frequent "carrier" of plasticity, the dislocations, are out of equilibrium defects which would not be present if a solid friction by solute atoms or crystalline potential was not preventing them from leaving the crystal. Similarly, fracture in metals is certainly irreversible, and thermodynamics is of little use if unloading a specimen does not lead to damage healing. As a result, while the main branches of physics, chemistry, mechanics contributed to the birth of the basic concepts of metallurgy, such as electronic structures of alloys, phase diagrams, diffusion processes, dislocations, cracks propagation and void growth, the modelling of the "real life" in any alloy requires a much more "craftsman approach" in which these basic concepts are used as tools to understand a specific system. As a colleague in mechanics always tells me, the annoying thing with metallurgists is that to any question they will answer "it depends"!

Does this mean that modelling in physical metallurgy is doomed to provide a collection of special cases? This is clearly not the case, and one of the purposes of this special issue is to exemplify for the reader who is not a metallurgist, that the tools to model solidification structures, or phase transformations in the solid state, or plasticity or fracture have reached a degree of maturity enabling them to provide both generic classes of behaviour, and to be applied to very specific situations in a way which aims at being predictive and quantitative.

Two key ideas are structuring the activity of modern physical metallurgy:

- Composition of an alloy does not tell the whole story: there is an intermediate scale of arrangement of atoms, called "microstructure", between the nanometer and a few microns, which depends on the thermodynamic properties of an alloy, and on its thermomechanical treatment, and which controls the macroscopic properties. One of the aims of physical metallurgy is to understand the processes, and to quantify the kinetics and the dimensions of the microstructures emerging from processes which, most of the time, are far from thermodynamic equilibrium.
- The structural defects present in metals and alloys, which can be seen as a departure from a periodic arrangement, whether these are point defects (vacancies or interstitials), line defects (dislocations) or planar defects (grain boundaries or interfaces), play a crucial role in the understanding of the influence of microstructure on macroscopic properties, an especially on mechanical properties such as plasticity and fracture.

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These two ideas are implicitly or explicitly present in any attempt to model the macroscopic behaviour of metals and alloy having undergone a history of thermomechanical treatment. Due to the complexity of the questions addressed, the physical metallurgist is forced to simplify his model down a caricature of reality, but a caricature which still contains the essential physics.

In order to answer to questions such as:

- what is the microstructure merging from a solidification process?
- what is the size and the volume traction of precipitates when an alloy is quenched below the solubility limit given by the phase diagram?
- what is the threshold at which dislocations move and multiply and how do they accumulate in the materials by mutual interaction or interaction with other defects?
- what are the mechanisms which lead to final fracture of a metal?

one has to consider simplified situations in which one mechanism is dominant, and from there to address the more and more complex interplay between the various elementary processes.

The leitmotiv of physical metallurgy is in the title of this special issue – changing scales: from the process parameters which are controlled at the macro scale, predict the microstructural features, and from the microstructural features predict the macroscopic mechanical properties. In the last decades, an increasing role of computer simulations and more generally, of "numerical metallurgy" has provided a new "modelling tool" for the metallurgist. The reason for this development, beside the increasing power of computers, is precisely because of the very nature of the problems addressed: very often a collective behaviour of defects is observed (such as in grain growth, or in dislocation patterning), very often the interactions are long ranged (as with dislocations or cracks), very often moving interfaces undergo morphological instabilities or kinetic transitions.

All these situations are ideal playgrounds for computer simulations, and the present issue provides a selection of examples of "numerical metallurgy" corresponding to some of the issues currently under investigation in the community.

- The metallurgist would like, for purposes of alloy design, to be able to go from atomistic calculations to phase diagrams [2];
- The metallurgist would like to understand the microstructures emerging from an incursion in a two phase region of the phase diagram, either via solidification [3] either via a diffusion controlled precipitation [4–6], or an interphase migration initiated from existing boundaries [7], or via a global evolution of the grain structure [8];
- The metallurgist would like to understand the collective behaviour of dislocations, these strange out of equilibrium linear defects with long range elastic interaction, and an annoying propensity to annihilate, multiply, react [9,10], and which are responsible for plasticity in many situations [11];
- The metallurgist would like to understand the global mechanical behaviour of an assembly of grains, each of them having an anisotropic plastic behaviour leading to incompatibility stresses. This concern, they have it in common with geologists interested by the behaviour of rocks [12];
- The metallurgist would like to predict the mechanisms leading to the final fracture of metals and alloys, whether plasticity plays a dominant role, such as in ductile fracture [13] or the fracture elementary process is the opening of crystallographic free surfaces as in brittle fracture [14].

These questions are a selection of problems, still open, visited by generations of metallurgists, in which the use of computer simulation has brought a new insight. They are by no means a complete picture of the field: for instance, we have limited ourselves in this selection, to situations involving condensed states of matter: vapour deposition is another story. We have limited our selection to mechanical properties: similar issues exist for the prediction of coercivity in magnets, of critical currents in superconductors. We have dealt with plasticity or textured materials, but not with the development of textures, either by deformation or by solidification, we have not addressed important topics such as irradiation damage in which computer simulation is the key modelling tool, or corrosion in relation with microstructure for which the modelling approach is still in its infancy. The aim of this issue was not to be exhaustive, but to provide an insight into a branch of metallurgy, computer simulation of scale transitions, which is extremely active.

Does it mean that the "back of the envelope calculation" has disappeared from the landscape of modelling activities in physical metallurgy? Certainly not, and one can bet that this art of modelling complex phenomena using very simple analytical models which was the rule in the beginning of modelling in metallurgy will remain an extremely fruitful approach to physical metallurgy. To paraphrase Warren Buffet "it's better to be approximately right than precisely wrong" [15]. Simulations give new insight into the type of problems listed above, where the collective behaviour is a key feature, where the transition from the atomic scale to the macroscopic scale is the ultimate goal. We may be fascinated by this new approach just like a child is fascinated by a new toy. But clearly the full program of "changing scale" can be carried out with computer simulations only on systems which are extremely simplified, and one still needs the prism of simple analytical modelling, either to capture the possible generality of a computer simulation, or to provide to the upper scale the information given by a simulation at the lower scale, in a usable form. Far from being replaced by computer simulations, analytical models have a new play ground here, since they are very often the link between simulations on idealised systems, and experiments

on real ones: by the art of simplification of a complex reality into a schematic description which retains the main features, without sinking into the irrelevant details, analytical approaches remain, in spite of the progresses in simulations, and may be even more because of the progresses in simulations, the best bridge between virtual numerical systems and real physical alloys.

Yves Bréchet
SIMAP, Grenoble-INP, BP75, 38402 St Martin d'Hères cedex, France
E-mail address: yves.brechet@simap.grenoble-inp.fr

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