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Scripta Materialia 68 (2013) 17–21
Scripta MATERIALIA
www.elsevier.com/locate/scriptamat

Viewpoint Paper

Diffusion as a method for producing architectured materials

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Available online 9 August 2012

Abstract—We describe the use of controlled diffusion treatments to arrange the distribution of alloying elements within a material. The Fe–C system is particularly interesting because of the strong effect of carbon on the mechanical properties and phase stability of steel. We demonstrate, through multi-step treatments, both one-dimensional and two-dimensional distributions of carbon within steel. A sample two-dimensional architecture is prepared and characterized to demonstrate feasibility. We briefly introduce a global optimization algorithm as a method for computationally optimizing treatment schedules.

Keywords: Functionally graded materials (FGM); Multilayers; Bulk diffusion; Global optimization

1. Introduction

Diffusional heat-treatments have been employed as a means of locally changing the chemistry and electronic properties in the semiconductor industry for over 40 years. In comparison, using similar treatments to create variations in mechanical properties has been largely overlooked and, until recently [1], has been confined to modifying surface properties of materials. In this contribution, we examine the possibility of using diffusional heat-treatments to introduce a controlled spatial distribution of an alloying element throughout the bulk of a material, so as to produce a desired adjustment in material properties. This idea of creating compositional heterogeneity in a material on a scale larger than the microstructure, with the express goal of optimizing specific properties, is relatively new in the materials/mechanics sphere and falls under the umbrella term "architectured materials" [2]; because our material is processed by diffusion and has gradually varying composition, we are preparing a specific class of architectured materials known as compositionally graded materials (CGMs). In our materials, the architecture comes about from the new length scale introduced by the diffusion treatments. The addition of features on this length scale might confer benefits on the material that are not superficially obvious. For instance, in these materials, the ductility has often been documented as exceeding that which is predicted by a simple mixing law. This behavior has been observed both in materials with very sharp interfaces (composites) [3] and gradual interfaces (CGMs) [4]. Furthermore, as an example that is less well known, the resistance of a material to crack propagation depends on both the yield stress gradients and on the stiffness gradients in the material [5], thus giving us the potential to engineer spatially varying resistance to fracture. In more general terms, we can identify other potential engineering targets for these architectured materials, including: work hardening rate, kinematic hardening and macro-internal stress distributions—all of which can be affected by the presence of composition gradients. For these reasons, we can see that taking into account properties that arise from structures on this scale can be of significant advantage to engineers.

The approach we discuss for fabricating these architectured materials is general and could be applied to a wide range of material systems. In what follows, the Fe–C system is used as a model system because of the dramatic effect that carbon has on the phase stability and mechanical properties of steel [6], as well as the ease with which the carbon can be introduced into, and removed from, the steel [1]. We demonstrate that it is possible to control the volume fraction and distribution of the reinforcement phase as well as the strength and presence/absence of the interface between the matrix and reinforcement. The discussion is divided into three parts.

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http://dx.doi.org/10.1016/j.scriptamat.2012.08.004

The first is focused on possible spatial distributions of the alloying element which could be obtained by thermal treatment. Next, we discuss the possibility of using phase transformations to enhance the contrast between the matrix and reinforcement phase. Finally, experimental results are presented to demonstrate the feasibility of this approach.

2. Control of the diffusion profile

The basic diffusion treatment needed to produce architectured steels is essentially that used for existing industrial gas-carburizing processes. Carbon is introduced into, or removed from, the steel using a carrier gas, which is, in the simplest case, a mixture of methane and hydrogen, or carbon monoxide and carbon dioxide. The composition of the gas controls the chemical potential of carbon at the surface of the steel. If the chemical potential of carbon in the gas is higher than that of the steel, carburization takes place; if the reverse is true, the steel is decarburized. Thus the gas ratio is a key processing parameter. A second processing parameter is temperature, which controls the rate of carbon diffusion in the steel; this, combined with time, determines the extent of diffusion. Diffusion masks could also be introduced as a means of introducing complex spatial distributions of carbon. By controlling the above-mentioned parameters, it is possible to produce a wide range of architectures ranging from simple multilayer structures to complex two- and three-dimensional patterns. Some of the carbon concentration profiles that could be readily produced in a square-cross section are shown in Figure 1.

The use of thermal treatments to produce composition gradients has several limitations. A major limitation is that the diffusion profiles produced during a given step will relax during subsequent processing steps. Similarly, sideway diffusion can take place below the masked regions and reduce the "sharpness" of the pattern. To appreciate the seriousness of these limitations, it is sufficient to consider the case of a multilayer structure produced by a sequence of carburizing and decarburizing steps. The concentration profile obtained in the thickness direction is not a sinusoidal one; rather it is an exponentially decaying, and broadening sine function. A second practical limitation is that performing the necessary heat-treatments for a given structure increases in difficulty dramatically as the scale and contrast of the patterns becomes finer; the most notable of these are the rapid treatment times required for small features and the extreme gas ratios required for high contrast.

We have previously mentioned the motivations for producing these architectured materials, namely the optimization of specific material properties. Additionally, the space of possible structures has been demonstrated to be very large. Therefore, a key requirement in the future of these materials is a method of optimizing a processing route to give a desired distribution of alloying elements, while keeping the previously discussed physical limitations in mind. One such global optimization algorithm is called a genetic algorithm. We have chosen this type of algorithm because of its decent performance over a wide range of optimization problems [7]; however, it is of note that many different global optimization algorithms exist, some of which may have improved performance for this particular problem [7]. A genetic algorithm can be most easily understood by thinking of its real-world, analogue evolution. In essence, the algo-

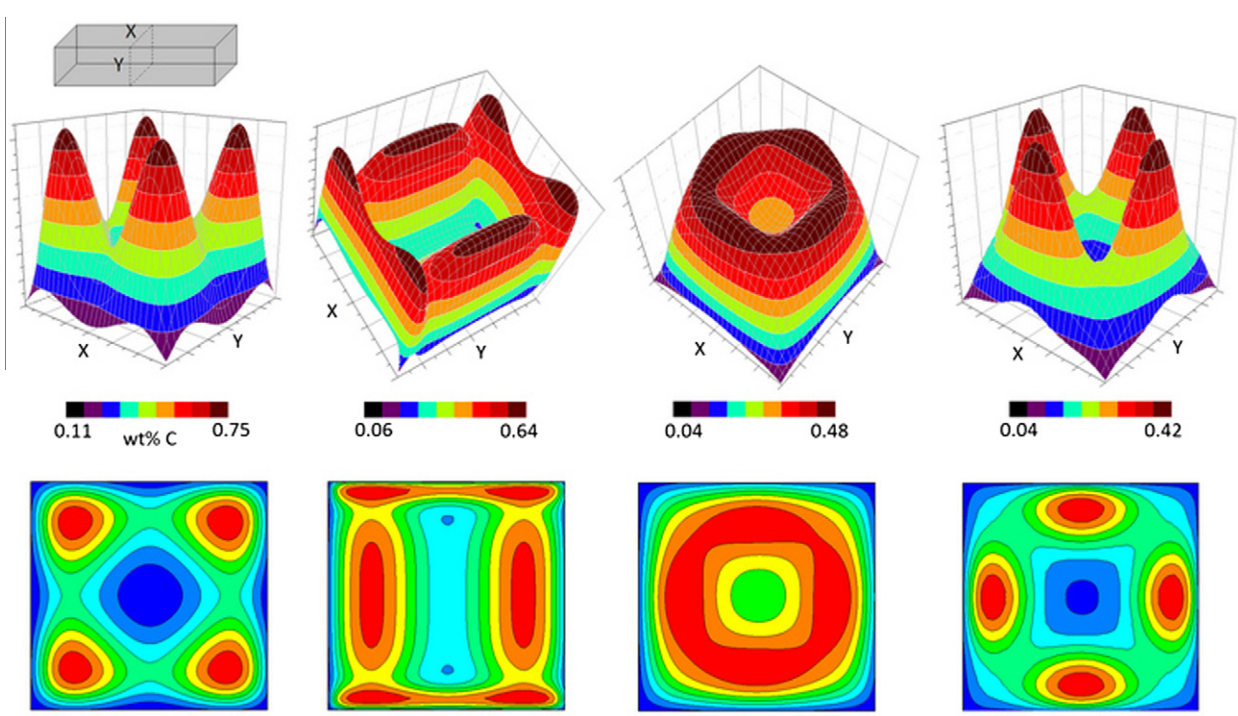

Figure 1. Two-dimensional distributions that can be produced by using diffusion on square cross-sections while using masks. Each pattern was made via a succession of processing steps involving changes in mask positions, and carrier gas ratios.