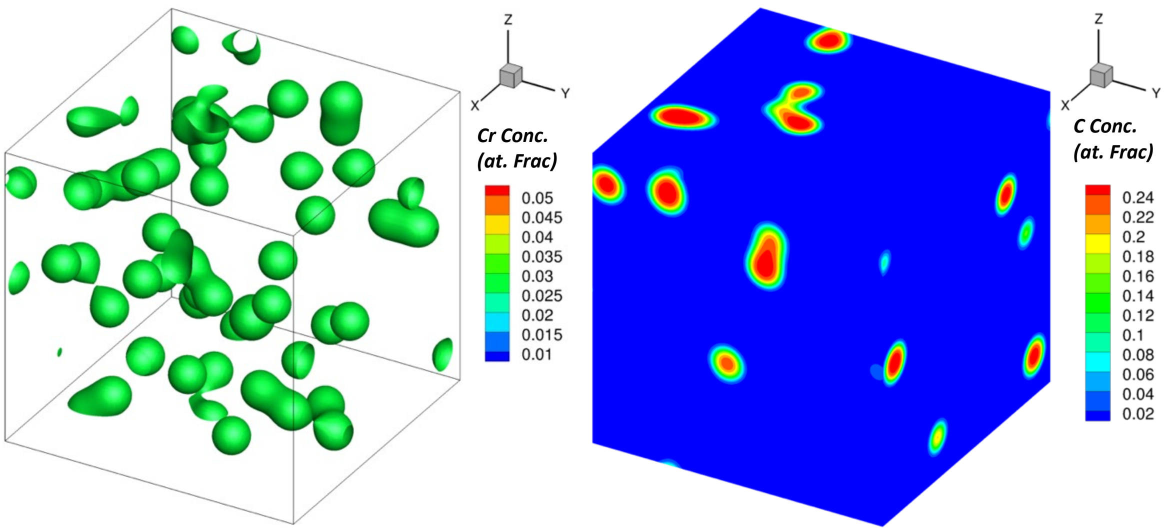
High Performance Computing to Quantify the Evolution of Microscopic Concentration Gradients During Flash Processing

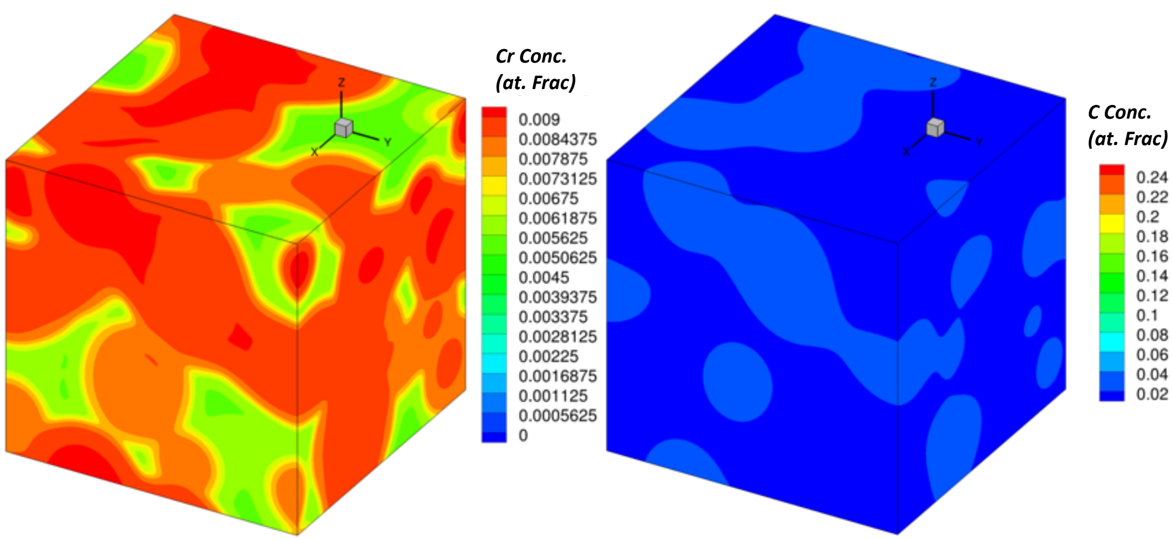
Steel used in impact loading applications require a combination of high strength and high ductility. The microstructure of the steels that meet this criterion are made up of structural units called martensites (phase) and bainites (constituent) that impart the required hardness to the steel. These hard phases and constituents are mixed in with a controlled amount of a third phase called "retained austenite" (RA) that allows the steels to possess sufficient toughness in addition to the strength. A class of steels called Advanced High Strength Steels (AHSS) have been under development by major integrated steel companies over a decade to target applications both in defense and transportation sectors. Flash Steelworks, Inc., (formerly known as SFP, LLC) has developed over the years, a very cost-effective process called Flash annealing, where strips of conventional carbon steels and low alloy steels are subjected to a rapid thermal cycle through induction heating followed by rapid cooling. During this process, phases in the steel such as ferrite, carbide and a combination of these two phases called pearlite dissolve to produce the austenite phase. In conventional heat treatment processes, the steel part is heated to the high temperature austenite field for long periods to allow complete dissolution of the ferrite and carbide phases and complete homogenization of the austenite composition. This is followed by rapid cooling (quenching) to produce a uniform distribution of martensite / bainite. However, in the Flash annealing process the residence time in the austenite field associated with the thermal cycle is such that the above processes do not go to completion, resulting in residual carbides and compositional gradients in the austenite at the microstructural length scale. During subsequent rapid cooling, the austenite phase with composition gradients produces a heterogeneous distribution of martensite, bainite and RA. The formation of martensite and bainite does not require extensive diffusion of the alloying elements in the steel. The ease with which they form depends mainly on the local steel composition and the temperature during cooling. The combination of strength and ductility in the final steel microstructure is determined by the level of heterogeneity in the distribution of martensite, bainite and the RA, which, in turn, is governed by the local composition gradients produced during the heating cycle.

The focus of the HPC4EI project was to develop a fundamental understanding of the development of local composition gradients in the steel when subjected to thermal cycles characteristic of Flash annealing. Specifically, the initiation of austenite formation (nucleation) from the dissolving carbide phase in the ferrite base, and its growth during rapid heating was simulated using a technique called the phase-field approach using high performance computing (HPC) that allowed large, three-dimensional simulations to be performed with a high spatial resolution so that the gradients could be captured accurately. An in-house developed phase-field code called MEUMAPPS (Microstructure Evolution Using Massively Parallel Phase-field Simulations) was used in the HPC simulations.

Figure shows the initial structure of the steel consisting of a base phase (matrix) ferrite in which spherical carbide particles are randomly distributed. Such microstructure are obtained through a prior heat treatment called spheroidization. A steel containing iron, chromium and carbon, proposed by Flash Steelworks was used in the simulations. The ferrite phase is lean in carbon and chromium while the carbide is rich in chromium and carbon. During rapid heating the austenite phase nucleates at the interface between ferrite and carbide, followed by the dissolution of the carbide in the austenite. This is followed by the growth of the austenite phase with a composition gradient that depends on the thermodynamic properties of the alloy. The simulations were able to capture the extent to which these changes occurred corresponding to various thermal cycles provided by Flash Steelworks.



Initial microstructure consisting of spherical carbides in a ferrite matrix.



Final microstructure after Flash thermal cycle showing composition gradients in chromium and carbon.

Reference

B. Radhakrishnan, Y. Song, S. Gorti and G. Cola, "High Performance Computing to Quantify the Evolution of Microscopic Concentration Gradients During Flash Processing", ORNL/TM-2022/2511, CRADA/NFE-19-07529, August 2022.