NOMATEN SEMINAR

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Challenges and advances in computational materials design

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Abstract: Over the last ten years, new methods have emerged that have led to significant acceleration in the field of alloy development. In particular, using high-throughput calculations from the early stages of development, new digital alloy design methodologies enable the development of alloys with multiple optimised characteristics in terms of thermomechanical properties (strength, creep, etc), chemical properties (oxidation) or other properties such as density, cost, etc. The approach used is that of "theoretical combinatorial metallurgy". It is based on models that can predict the characteristics of interest as a function of the composition. Hence, extensive use of models such as the CALPHAD thermodynamic models, but also Machine-Learning-type regression models, enables to assess the looked-for properties by exploring the full theoretical composition domain. One of the problems to deal with is the gigantic number of possible compositions: for example, with a dozen alloying elements, like in most complex industrial alloys, and around fifty possible concentration levels for each of them, the number of potential alloys is 5012, i.e. more than 2.1020 alloys! It is therefore impossible, even by calculations, to explore systematically the entire compositional range. Reducing the composition domain explored (concentration ranges, number of elements, number of levels) to authorize brute-force calculations, or using optimization algorithms, such as genetic algorithms are the two strategic solutions. In fact, optimization algorithms enable to perform an "intelligent exploration" of composition space, gradually converging, through iterative processes, towards the Pareto front, i.e. the only areas of the composition domain that are "interesting" in terms of the defined objectives.

Bio: Dr Clara DESGRANGES, Senior Expert in Materials Science at CEA-Saclay received a degree in Materials Engineering from FIUPSO in Orsay in 1995 and a PhD in Metallurgy and Materials from Paris XI University in 1998. Her doctoral thesis at Physical Metallurgy Department at CEA in Saclay focused on understanding transmutation effects in neutron-absorbing alloys, and was awarded by Jean Bourgeois prize of the SFEN (Société française d'énergie nucléaire). In 1998, she carried out a post-doctoral project for Arcelor group at the research center in Maizières-lès-Metz on the kinetics of precipitation in IF (Interstitial Free) steels. In September 1999, she joined CEA Saclay as a research engineer in the Corrosion Department. Her area of research focused then on HT oxidation by gas and the modeling of high-temperature oxidation phenomena for nuclear applications (waste, HS tubes, etc.) and non-nuclear applications such as interconnectors for SOFC fuel cells. In 2013, she became Head of the Modeling, Thermodynamics and Thermochemistry Laboratory within the Corrosion Department, and further specialized in the use of CALPHAD-type thermodynamic and kinetic modeling tools. In June 2016, she joined the industrial 's research center of Safran group (international high-technology group operating in the aviation -propulsion, equipment and interiors) as a Metallurgy Senior Expert in the Materials and Processes Department. She has built up and managed projects in the fields of Digital Metallurgy, Innovative Materials (HEA, thermoelectric ...) and High-Temperature Corrosion for Aeronautics applications. In September 2022, she returns to

the CEA Saclay with a specific mission on Numerical Alloy Design for the Low Carbon Energy sources Institute (ISAS).