PhD Thesis 2019-2022

DEVELOPMENT OF REACTIVE POWDERS FOR POWDER METALLURGY

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Context: Contemporary additive technologies are based on a principle of layer-by-layer selective sintering/melting of polymer, metallic or ceramic powders. Selection of refractory powders (metallic or ceramic) are limited by temperature achieved in the zone of local heating that must be close to the melting point of the powder particles. The most powerful, advanced 3D-printers, working on the base of selective laser sintering (SLS) and selective laser melting (SLM), are able to use Ni-, Al-, Ti-based metallic alloys or steels. for obtaining stronger and more temperature-resistant items in comparison with polymer models. However, polymer binder still often has to be used together with the metallic powders and then must be removed by annealing in the furnaces. The development of a new type of powders for 3D sintering such as **reactive particles** (RP) is a real challenge.

Research project: This research is conducted with one major aim: to demonstrate the feasibility of producing RPs with a well-controlled microstructure that are directly suitable for additive technologies. Concerning the preparation of RPs, ball milling will produce nanostructured composites with the size of the structural components in the range 10-100 nm. The contact area between elements increases significantly and the interfaces formed during HEBM in inert atmosphere are clean from oxide films. Our study will aim at determining the degree of alloying between metallic powders during HEBM as a function of the process conditions (milling time, energy, mode). Depending on the energy injected in the system during the HBEM process, two major microstructures are expected for the composite powders: core-shell systems and lamellar composites. Both will exhibit a specific reactivity that has to be investigated in order to identify the preferable system for spark plasma and selective laser sintering applications.

The experimental investigations will be carried out together with appropriate modeling. In parallel to the experimental work, we will perform a detailed theoretical investigation based on a multiscale modeling of RPs. The modeling will combine different techniques including Molecular Dynamics (MD) simulations, Discrete Element Method (DEM) and mesoscopic modeling. MD simulations will be developed in order to follow the elemental mechanisms governing the kinetics aspects at the microscopic level, such as friction between metallic particles, diffusion, creation of defects, local ordering, precipitation, local stress and reactive behavior due to laser initiation. For the first time, an atomistic scale counterpart of the laser induced sintering will be formulated. This multiscale modeling will investigate the influence of the nanostructure of RP on its reactivity and its response to laser ignition. Our approach will provide new tools to shorten the conception of RPs and reduce the cost of their elaboration. The control of the process-microstructure relation should help us to overcome technological bottleneck and obtain tailored materials with improved properties. An important issue is to obtain items produced by additive technologies with good corrosion resistance and mechanical properties.

International context: This project is part of the collaborative research project PHC Kolmogorov between the ICB lab (uB) and the scientific research center ñFunctional Nanoceramicsò at NUST ñMISiSò (Moscow). The student will have the opportunity to collaborate with the incoming researchers. In addition, he(she) will have the opportunity to visit the Russian lab.

Type of project: theory and experiment, modeling, molecular dynamics

Required knowledge: A basic knowledge in materials science and statistical physics is required. A skill in numerical methods and computational languages is expected. The candidate will learn the necessary tools to develop molecular simulations with open source software (LAMMPS). The scientific curiosity of the candidate will be appreciated.