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MOLECULAR DYNAMICS SIMULATIONS AS A TOOL FOR MATERIAL SELECTION IN METAL INJECTION MOULDING FEEDSTOCKS

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Abstract

Metal injection molding (MIM) is a technology used to produce small metal parts with complex geometries. MIM consists of (i) preparing a highly-filled feedstock of polymeric binder with metallic particles, (ii) shaping the feedstock by injection molding, (iii) removing the polymeric binder, and finally (iv) sintering the metallic particles to obtain a solid part. When developing new feedstock materials, it is important to understand the behavior of polymers close to a metallic interface, since the behavior of materials at the molecular scale strongly affects the properties of the feedstock at the macroscale. For example, the binder should have sufficient affinity to the metallic particles to prevent their agglomeration during the shaping process and prevent excessive geometrical distortion during the debinding process. One way to study the interfacial interaction is to use atomistic molecular dynamics (MD) simulations.

In this work, MD simulations were used to study the interactions and conformational characteristics of confined molten polypropylene (PP) chains between ferric oxide (Fe_2O_3) substrates. PP can be readily used as one of the main components of binder systems in MIM and Fe_2O_3 layers are always present on the surface of stainless steel powders. The simulations revealed that PP has a strong adsorption of chains on the surface of Fe_2O_3, since the local density of PP chains is higher closer to the interface. Moreover, the backbone carbon-carbon bonds of the chains preferably orient in the direction parallel to the oxide surface. The results confirm the applicability of PP as a backbone component in a MIM feedstock containing ferritic materials due to their good affinity.

References

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