ATOMISTIC SIMULATION OF METALS PRIMARY MICROSTRUCTURE FORMATION DURING RAPID CRYSTALIZATION

V. V. Dremov[1], P. V. Chirkov[1], R. M. Kichigin[1], A. V. Karavaev[1], E. B. Cherepetskaya[2], V. V. Cheverikin[2], V. S. Dub[3], I. A. Ivanov[2, 3], S. V. Salikhov[2]

[1]FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin», Snezhinsk, Russia

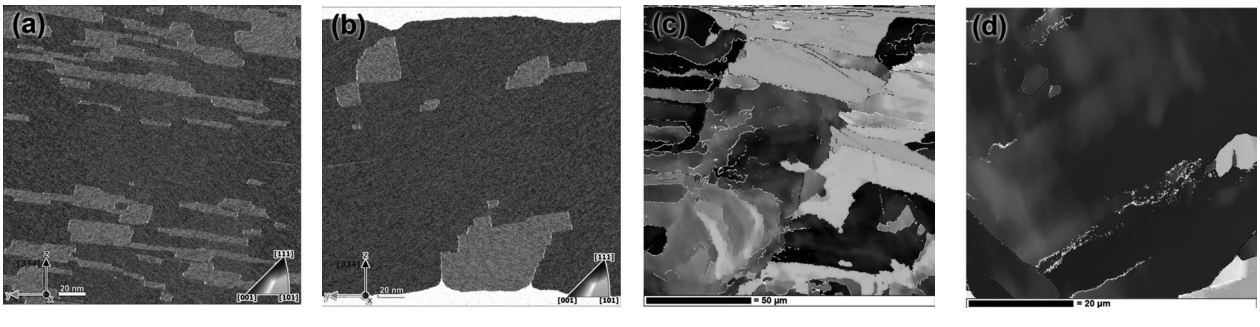
[2]NUST "MISIS", Moscow, Russia

[3]NPO "TsNIITMASh", Moscow, Russia

In additive manufacturing of metal parts using Selective Laser Melting (SLM), high temperature gradients and a small melt pool volume are achieved, bringing the process scale close to the capabilities of modern atomistic modeling methods. Present study employs atomistic modeling to investigate the microscopic mechanisms responsible for the formation of the primary microstructure during rapid melt crystallization [1]. The material selected for analysis is 316L stainless steel, which is widely used in SLM. It is demonstrated that the solidified material inherits defects from the substrate and develops new ones, which interact with the crystallization front, thereby defining the primary microstructure. In this work we explore the characteristics of crystallization in various crystallographic directions, the interaction of the crystallization front with grain boundaries (inherited from the substrate) and newly formed defects (twin boundaries), as well as the specifics of their formation. The resulting microstructure of virtual samples was compared with that of real SLM-produced samples analyzed via Electron Backscatter Diffraction (EBSD). The comparison revealed similarities in EBSD patterns, confirming the ability of molecular dynamics simulations to reproduce key microstructural features observed in SLM processes.

The calculations revealed the formation of multiple twinning planes during crystallization in the [111] direction. The average twin size is determined by the degree of undercooling the closer the crystallization temperature is to the equilibrium melting temperature, the larger the characteristic size.

The simulation also demonstrated the role of twinning in changing of the crystallization geometry front and shaping the primary microstructure. A comparison of the microstructure of virtual and real samples is presented in Fig. 1. The figure shows that the subgrain microstructure of the printed samples resembles that of the virtual samples, considering the scale difference associated with the crystallization rate.



a *b* *c* *d*

Fig. 1. Twinned structure of crystallized samples (EBSD analysis).

a, *b* – molecular dynamics simulation results; *c*, *d* – EBSD of real samples produced by SLM.
a, *c* – high crystallization speed; *b*, *d* – low speed

References

1. **Dremov, V. V.** Atomistic simulation of primary microstructure formation in metals during crystallization from the melt [Text] / V. V. Dremov et al. // Sci. Rep. 2024. – Vol. 14. – P. 28105.