11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

MULTISCALE MODELING OF SOLID-LIQUID INTERFACE ORDERING AND ITS EFFECT ON THE GROWTH KINETICS OF METALLIC ALLOYS

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Key words: *multiscale modeling, MD simulation, phase-field modeling, solid-liquid interface phenomena, growth kinetics, multiphysics problems.*

The structure and dynamics of solid-liquid interfaces remains an open question in condensed-matter science. Understanding these issues is of particular importance because of their crucial influence on various physical phenomena such as freezing, wetting, and capillary osmosis. We illustrate here how local ordering in a metallic melt (NiZr) transforms into a massive in-plane ordering at the surface of a crystal (bcc Zr) when the solute-centered clusters of the melt match the periodic potential of the crystal surface (Fig. 1). Our observations provide evidence for a strong link between the interface ordering and the short-range order (SRO) in the bulk liquid. In other words, what we observe are not only single 'liquid' atoms which mimic the periodicity of the crystalline wall without any relation to the local order of the melt, as reported until now in the literature. Rather, the liquid alloy rearranges the solid-liquid surface to develop (100) facets and then docks its trigonal prisms at them. Using a hierarchical multiscale modeling concept, by linking molecular dynamics (MD) simulation to phase-field (PF) modeling, allows to estimate quantitatively the influence of the surface effect on the growth kinetics [1]. 'Freezing' of the melt SRO at the solid-liquid interface is found to act against the crystallization. Furthermore, our study suggests a possibilty to give experimental evidence for the existence of the structural units of the melt by capturing them at suitable interfaces.

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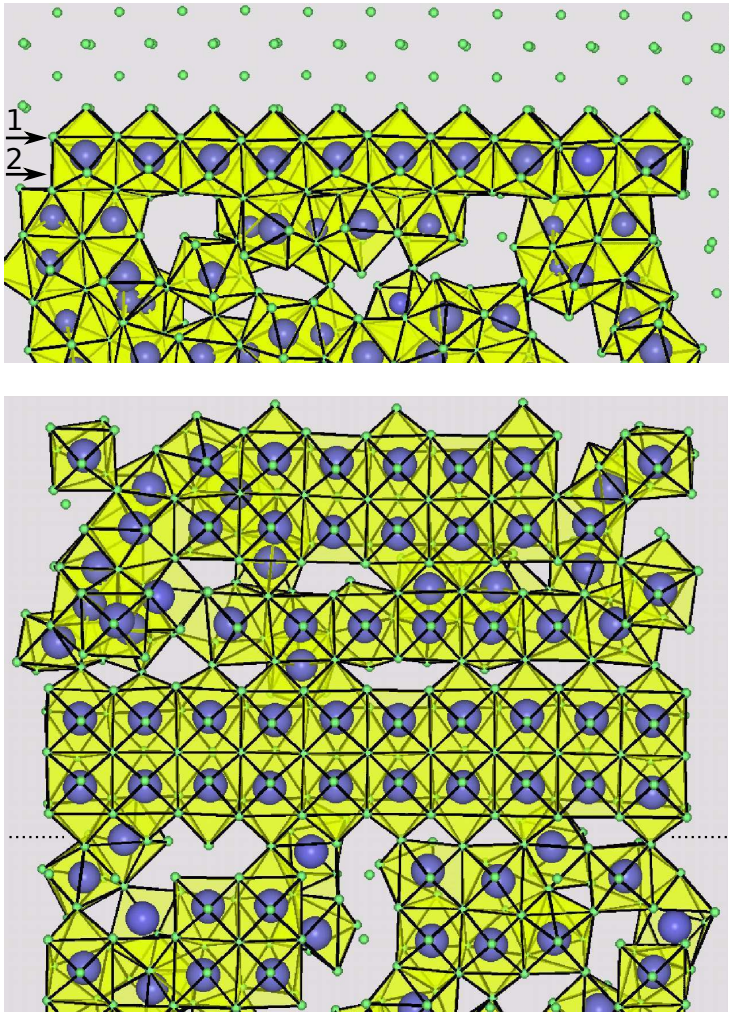

Figure 1: Top: Side view of a $[Ni_cZr_{1-c}]_{liquid}$-$Zr_{crystal}$ (100) interface at 1100 K. For clarity, Zr atoms are represented by small spheres. Each Ni atom is represented by its coordination polyhedron. The Ni-atom size scales with the distance from the drawing plane. The number '1' and '2' designate two different Zr-atom planes. Bottom: Top view of the interface. Zr atoms lying between the observer and the Ni-atom layer constitute the first two monolayers of the bcc substrate. A bottom view at the level of the dashed line gives the figure above. (From Ref.[1])