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Icosahedral Order in Undercooled Metallic Liquids - Impact on the Crystal Nucleation Barrier and Thermophysical Properties

KENNETH KELTON, Dept. of Physics, Washington University, St. Louis, MO 63130

Over a half-century ago, Charles Frank argued that metallic liquids could be undercooled because of developing icosahedral short-range order (ISRO) in the liquid that is incompatible with the translational periodicity of crystal phases. Our recent high-energy x-ray diffraction and nucleation undercooling studies of electrostatically levitated droplets of a Ti-Zr-Ni liquid produced the first experimental proof of this hypothesis. In addition to coupling to the nucleation barrier for the ordered phase, the icosahedral order can significantly influence the thermophysical properties of the liquid. A sharp decrease in the specific heat that is correlated with the growing ISRO indicates a rapidly decreasing configurational entropy in the liquid, at temperatures far above the glass transition temperature. Surprisingly, our studies demonstrate that ISRO is evident even above the liquidus temperature in the Ti-Zr-Ni liquid as well as in liquid Ni. It is significantly distorted in liquid Ti, consistent with an increasing importance of the covalent character of the 3-d bonding, which frustrates the development of ISRO. Supported by NASA under contract NAG8-1682, and by the National Science Foundation under grant DMR 03-07410.