Role of Hf on phase formation in Ti_{45}Zr_{38-x}Hf_xNi_{17} liquids and solids


Department of Physics, Washington University, St. Louis, MO 63130, USA

Hafnium and zirconium are very similar, with almost identical sizes and chemical bonding characteristics. However, they behave differently when alloyed with Ti and Ni. A sharp phase formation boundary near 18-21 at.% Hf is observed in rapidly-quenched and as-cast Ti_{45}Zr_{38-x}Hf_xNi_{17} alloys. Rapidly-quenched samples that contain less than 18 at.% Hf form the icosahedral quasicrystal phase, while samples containing more than 21 at.% form the 3/2 rational approximant phase. In cast alloys, a C14 structure is observed for alloys with Hf lower than the boundary concentration, while a large-cell (11.93 Å) FCC Ti_2Ni-type structure is found in alloys with Hf concentrations above the boundary. To better understand the role of Hf on phase formation, the structural evolution with supercooling and the solidification behavior of liquid Ti_{45}Zr_{38-x}Hf_xNi_{17} alloys (x=0, 12, 18, 21, 38) were studied using the Beamline Electrostatic Levitation (BESL) technique using 125keV x-rays on the 6ID-D beamline at the Advanced Photon Source, Argonne National Laboratory. For all liquids primary crystallization was to a BCC solid solution phase; interestingly, an increase in Hf concentration leads to a decrease in the BCC lattice parameter in spite of the chemical similarity between Zr and Hf. A Reitveld analysis confirmed that as in the cast alloys, the secondary phase that formed was the C14 below the phase formation boundary and a Ti_2Ni-type structure at higher Hf concentrations. Both the liquidus temperature and the reduced undercooling change sharply on traversing the phase formation boundary concentration, suggesting a change in the liquid structure. Structural information from a Honeycutt-Anderson index analysis of reverse Monte Carlo fits to the S(q) liquid data will be presented to address this issue.
Role of Hf on Phase formation in Ti45Zr38-xHfxNi 17 Ti45Zr(38-x)HfxNi17 Liquids and Solids


- Washington University in St. Louis, b-Army Lab USADOE, c-University of Massachusetts Amherst, d-NSA Marshall Space Flight Center, e-Iowa State University, f-Argonne National Laboratory

Introduction
- Initial studies revealed a sharp boundary in phase formation around 21 at% Hf (x=21) in the Ti45Zr38-xHfxNi17 system. In quenched alloys the i-phase forms below the boundary, while a 3/2 rational approximant to the quasicrystal forms above. In cast alloys, the C14 Laves phase forms below and a Ti2Ni-type (cF96) forms above. Further study of the liquid structure and evolution and the influence of Hf on phase formation and physical properties were studied using the Bimane Electro Static Levitation (BESL) technique [1].

Experimental methods
- High-resolution scattering data collected to 14.5 Å reverse Monte Carlo (RMC) simulation generates atomic configuration [7].
- Reliability parameter (RMC) from analysis used to quantify order in the RMC structures.
- HA index describes bonded neighbors of a root pair, i.e.,...

Quantifying structure
- Icosahedral or disordered icosahedral order is most prominent for all compositions.
- Local icosahedral order is increasing with...