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Thermodynamics and solidification of Ti-Ni-Cu-Nb alloys

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In this study, the solidification process of Ti52-xNi38Cu10Nbx alloys was analyzed from the perspective of thermodynamic simulations using Scheil and equilibrium calculators on ThermoCalc. Alloys with Nb additions of x = 4, 6, 8 and 10 at% were produced by arc-melting and the as-cast microstructures were evaluated by XRD and SEM/EDS analyses. By relating the experimental characterization of the as-cast structure with the simulation results, we aim to assess the role of Nb on the solidification process and the solute distribution in the studied Ti-Ni-Cu-Nb alloys. Both in Scheil calculator and XRD/SEM analyses, the observed phases were TiNi, ?-Nb, and Ti2Ni. Moreover, metallic Ti was observed in Nb10 alloy. Enrichments on the Ti content concurrent to decreases on the Ni content were observed in the Scheil calculation of all compositions when the formation of TiNi takes place. The chemical gradient of these two elements on liquid decreases with increasing Nb-alloy-content and the TiNi/?-Nb eutectic reaction takes place with lower Ni depletion. In turn, the formation of Ti2Ni, which occurs in regions with higher Ti enrichments and Ni depletion, becomes more difficult. This reflected in increasing ?-Nb and decreasing Ti2Ni volume fractions. By integrating the XRD peak areas under the indexed peaks of each phase and dividing them by the sum of all the integrated peak areas in a qualitative analysis, volume fractions of ?-Nb and Ti2Ni of 3% were obtained in the alloy with 4at% Nb while 15vol% and 1vol% were obtained, respectively, in the alloy with 10at% Nb. On the other hand, by evaluating the solute distribution from EDS results, it has been observed that Cu is always present as a solute, preferably in NiTi, whereas Nb precipitates as the BCC ? phase. In the intermetallic phases, coherent ratios are obtained in NiTi when Cu is considered a substitute for Ni, and Nb, for Ti. In Ti2Ni, the calculated ratios fit the stoichiometry the best when only Nb is considered a substitute for Ti. These results endorse that Nb occupy Ti sites in Ni-Ti intermetallic phases.