CALCULATION OF THE LATTICE PARAMETERS OF BETA-TITANIUM-ALUMINUM-RUTHENIUM SOLID SOLUTION ALLOYS

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In preparation for high temperature x-ray diffraction studies, the lattice parameters of the beta solid solution in the Ti-Al-Ru system were calculated as a function of composition and temperature. Two computational models were used. The first model incorporates the variation of beta-Ti lattice parameters as a function of temperature and takes into accounts for the paired interaction between each of the constituent atom types, Ti-Al, Ti-Ru, and Al-Ru, assessed from the previous experimental studies. Since the lattice parameter of beta-Ti-Al alloys has never been experimentally investigated, the Ti-Al interaction was determined through an extrapolation of experimental lattice parameter versus composition data for beta-Ti and gamma-TiAl. The second model predicts the lattice parameter through the modeling of the average interatomic spacing for solid solutions proposed by Moreen et al. (1971). The combined contribution from the pure components, Ti, Al, and Ru, and their pairs, Ti-Al, Ti-Ru, and Al-Ru, was accounted for. The change in lattice spacing for the structures with different co-ordination numbers was achieved through the application of experimental data, where available, or Goldschmidt's approximation. Evaluation of the two proposed models will be discussed in conjunction with the limited available experimental data. Suggestions on sources of error will be also given.