

Prediction of CCT Curves for Titanium Alloys Based on Energetics

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Efficient evaluation and development of heat-resistant titanium alloys requires not only experimental investigation, but also analysis and prediction of microstructural changes at high temperatures by calculation. The precipitation phenomenon of the second phase, which is important for many heat-resistant materials, is generally analyzed by the Langer-Schwartz theory¹⁾, etc. However, it is difficult to apply this theory to newly developed materials with little experimental data, because it requires the input of many parameters. In this study, we proposed a method to predict the precipitation of α -phase from β -supersaturated solid solution in practical titanium alloys based on energetics (and simple kinetics) using the minimum necessary known basic parameters. Especially, we attempted to evaluate the continuous cooling transformation (CCT) curves of the α -phase by calculation to predict the precipitation in the super thermal field during additive manufacturing.

In this study, decrease in temperature at a constant rate was approximated by the temperature change with a staircase combination of minute time isothermal processes²⁾. The total diffusion distance of atoms in continuous cooling process was calculated by integrating the diffusion distance for a minute time using the diffusion coefficients at each temperature. Estimating the size of the spherical embryo that can be precipitated by the diffusion distance, the free energy of the system in the coexistence of β -matrix and α -embryo was expressed as the sum of the chemical free energy G_0 of the coexisting two phases and the interfacial energy E_{intf} due to the interface between β/α phase. In this case, G_0 and E_{intf} were not evaluated separately, but were optimized by Newton-Raphson method to minimize the sum of the energies by varying the concentrations of the coexisting phases, which are common variables for these energies. At each step change in temperature during the continuous cooling process, the energy coexisting β -matrix and α -embryo was evaluated and compared to the energy of β -supersaturated solid solution at that temperature. And it was assumed that α -phase was precipitated under the temperature and time conditions where the former energy was lower. These calculations were performed at different cooling rates, and the CCT curve was predicted by plotting the precipitation starting time of α -phase and comparing it with the experimental results³⁾.

Fig. 1 shows the CCT curves of a Ti-6Al-2Sn-4Zr-2Mo (mass%) alloy cooled from 1273 K at a constant rate.

The red and black dashed lines are the calculated and experimental results³⁾, respectively. The calculated CCT curve of α -phase reproduced the precipitation around 10 s at 1200 K. However, the predicted precipitation start-time overestimated temperature dependence than the experimental results. Fig. 1 could be calculated only from the chemical free energy, interfacial energy density between β/α phase, molar volume, and diffusion coefficient obtained from a commercial phase diagram calculation software and references. Even for newly developed materials without detailed experimental data on precipitation, CCT curves could be obtained roughly by this calculation method and existing basic data (and their extrapolation) for only a few minutes with a personal computer.

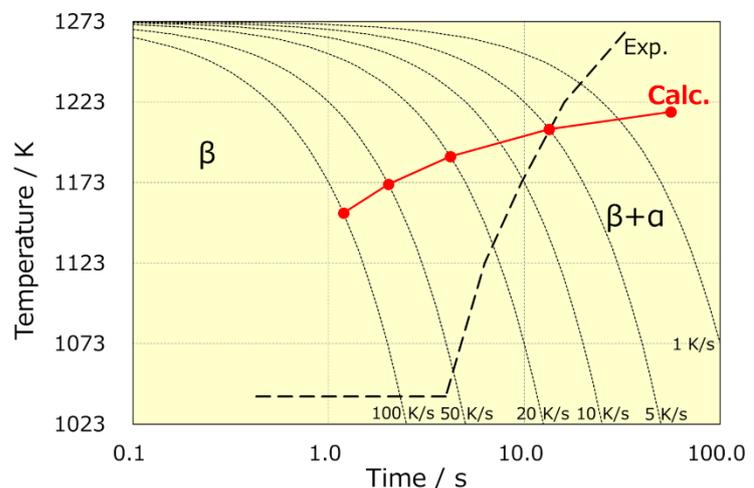


Fig. 1 Calculated and experimental³⁾ continuous cooling transformation curves of α -phase in practical heat-resistant Ti-6Al-2Sn-4Zr-2Mo (mass%) alloy.

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