Nucleation and transition sequences of TCP phases during heat-exposure in a Re-containing Ni-based single crystal superalloy

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Abstract: The nucleation and transition sequences of topologically close-packed (TCP) phases in a Re-containing Ni-based single crystal superalloy were systematically investigated using in-situ transmission electron microscopy (TEM) and three-dimensional atom probe technology (3D-APT). During the initial stage of heat-exposure at 1100 ° C, the TCP phase forming elements (Re, Co, Cr, etc.) segregated at the γ/γ' interface near the γ matrix side to provide the concentration undulations for the nucleation sites of TCP phases, following which the σ and P phase coherently nucleated along the $(1\bar{1}\bar{1})\gamma$ and $(022)\gamma$ planes from the γ/γ' interface near the γ matrix side, respectively. With prolonged heat-exposure time, transitions from σ phase to P phase, σ phase to μ phase, and P phase to μ phase occurred. Besides, the orientation relationships of TCP phase intergrowth structures indicated that the P phase grew along the $(\bar{1}01)\sigma$ plane of the σ phase by co-lattice precipitation, meanwhile the μ phase grew with smaller lattice misfits along the $(0\bar{4}0)\sigma$ plane of the σ phase and the (400)P plane of the P phase. Additionally, the result by first-principles calculation evidenced that the μ phase had the lowest system energy to make the transition of σ phase and P phase to μ phases inevitable, therefore, the TCP phase ultimately existed as the most stable μ phase. Finally, the transition sequences of TCP phase during heat-exposure could be summarized into three types: γ matrix→σ→μ, γ matrix→P→μ, and γ matrix→σ→P→μ.

Keywords: Ni-based single crystal superalloys; TCP phase; Nucleation; Intergrowth

1 Introduction

Ni-based single crystal superalloys are widely used in the manufacture of hot-end components for advanced aero-engines due to their excellent high-temperature mechanical properties, structural stability, oxidation resistance, and creep resistance[1-4]. With the development of aero-engines, the requirements for the high-temperature mechanical properties of Ni-based single crystal superalloys are constantly increasing. Generally, the temperature-carrying capacity of superalloys can be improved by the addition of refractory elements such as Re, Cr, and W[5-7]. However, the increase in the content of refractory elements leads to an increased tendency for precipitation of the TCP phase[8-15]. TCP phase is a brittle phase, which not only easily becomes the crack source and expansion channel of alloy fracture, but also greatly weakens the solid solution strengthening effect of superalloys, thereby impairing its creep property and seriously threatening the safety of aero-engine[16-20]. Therefore, the study of the TCP phase has become an important topic to be solved in the development and application of Ni-based single crystal superalloys.

In this paper, the nucleation and intergrowth behavior of TCP phases in a Re-containing Ni-based single crystal superalloy was systematically investigated by in-situ TEM and 3D-APT to clarify the nucleation site, the orientation relationship between the TCP phase and γ matrix, and the transition sequences of TCP phases during heat-exposure at 1100 ºC. Furthermore, the first-principles calculation based on the density functional theory (DFT) about the system free energies of different types TCP phases were also used to further elucidate the transition mechanisms. The results provided insight to the nucleation and growth of TCP phases, and would also help to offer the theoretical support for the composition design and microstructure regulation of advanced Ni-based single crystal superalloys.

2 Experimental section

In this work, the nominal composition of the

experimental superalloy was as follows (wt.%): 14.0 Co, 6.0 Al, 19.5 (Cr+Mo+W+Ta), 0.1 Hf, 5.4 Re, and the balance Ni. The single crystal bars with orientation [001] were prepared by liquid metal cooling directionally solidification furnace. The schematic diagrams of the directional solidification devices were shown in Fig. 1.

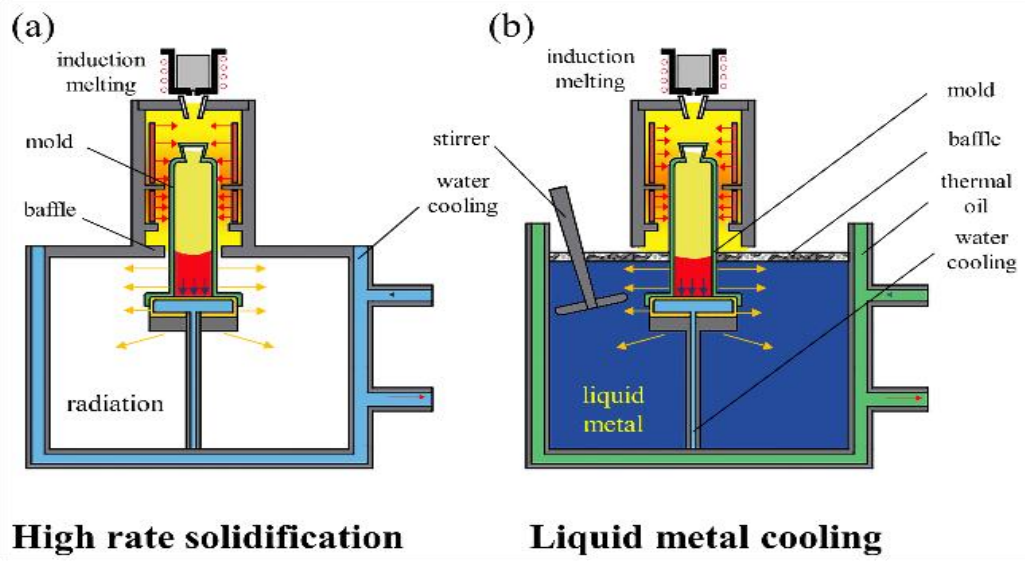

Fig. 1: The schematic of the high rate solidification furnace (a) and liquid metal cooling furnace (b).

3 Results and discussion

3.1 Nucleation of TCP phases

The microstructure and component distribution of the experimental alloys after heat-exposure at 1100 °C was analyzed by TEM and 3D-APT, and the results were shown in Fig. 1. After a short heat-exposure, it could be found that the TCP phase preferentially nucleated from the side near the γ/γ′ interface near the γ matrix (Fig. 2a). By characterizing the TCP phases, it was demonstrated that the preferentially precipitated TCP phases were the σ and P phases, which exhibited the specific co-lattice relationships with the γ matrix. In addition, the results of 3D-APT (Fig. 2b) indicated that the TCP phase-forming elements, such as Re, Co, and Cr, were segregated at the γ/γ′ interface near the γ matrix side during heat-exposure. Therefore, it could be concluded that the segregation of the σ and P phases forming-elements at the γ/γ′ interface near the side of the γ matrix provided concentration undulation for the nucleation of the σ and P phases, and the γ matrix could provide nucleation sites for the σ and P phases to stabilize the nucleus and reduce the critical nucleation size, thus promoting the nucleation of the σ and P phases on the γ matrix near the γ/γ′ interface.

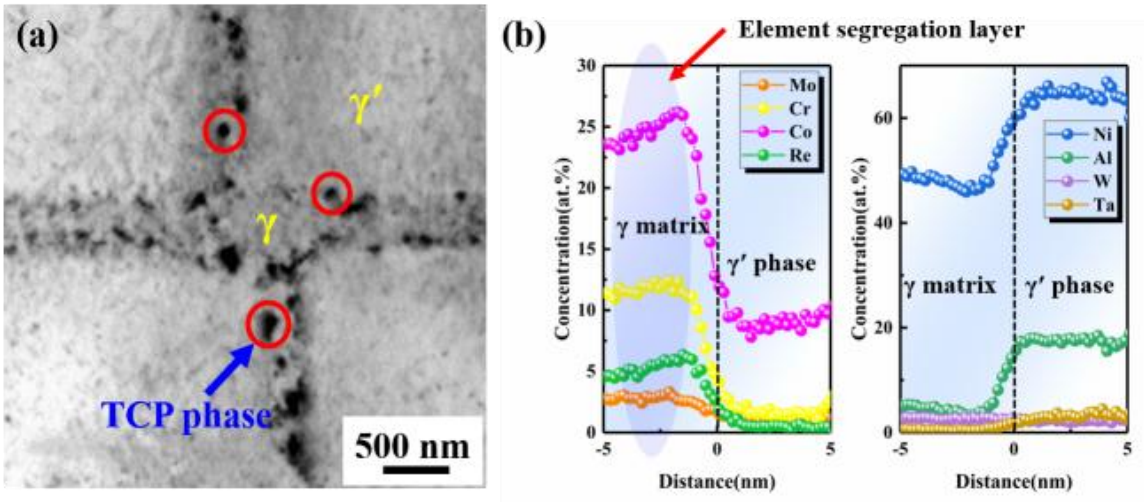

Fig. 2: The bright field image of the alloy (a) after heat-exposure at 1100 °C for 2 h was investigated by TEM. The plots of the variation of the concentrations (b) as a function of distance away from the γ/γ' interface in the experimental alloys during heat-exposure at 1100 °C for 100 h.

3.2 Transition behavior of TCP phases

It was known that different types of TCP phases could transform during the growth during heat-exposure at 1100 ºC, thus further analysis was done by TEM to target the transition sequences of the TCP phase, and the result was displayed in Fig. 3. As shown in Figs. 3a_1-c_1, σ/P, σ/μ, and P/μ intergrowth structures were present during heat-exposure for different times, and computational comparison and calibration of their SAED patterns (shown in Figs. 3a_2-c_2) showed that the intergrowth structures of TCP phases had a certain orientation relationship. After calculating the misfit lattices of the specific interface, the σ/P, σ/μ, and P/μ interfaces might be a coherent lattice matching with the misfit δ of 1.70%, 7.41%, and 4.23%. Besides, the lowest system energy of the μ phase calculated by DFT (as shown in Fig. 4) caused both σ phase and P phase to eventually transform to the μ phase. With the further extension of the heat-exposure time, the TCP phase ended up in the most stable μ phase.

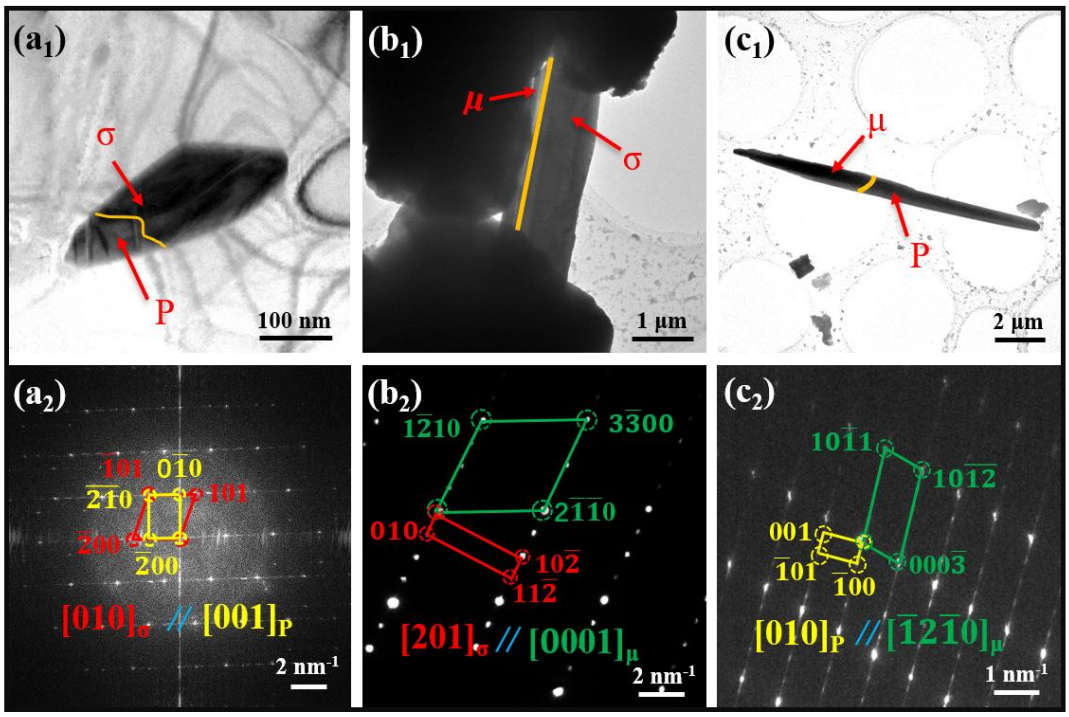

Fig. 3: The Bright field TEM micrograph of σ /P (a1), μ/σ (b1), and μ/P (c1) intergrowth structures. (a2-c2): the SAED patterns of σ /P, μ/σ, and μ/P intergrowth structures.

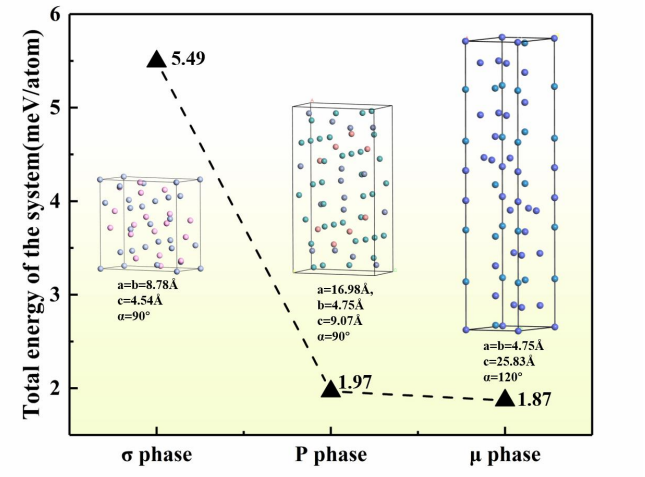

Fig. 4: The system energy of σ phase, P phase, and μ phase calculated based on the first principles calculations.

4 Conclusions

1. During heat-exposure at 1100 °C, TCP phases preferentially nucleated from the γ/γ′ interface and close to the γ matrix side due to the concentration undulations provided by the segregation behavior of TCP phase forming elements (Re, Co, Cr, etc.) at the γ/γ′ interface close to the γ matrix.
2. The transition sequences of the TCP phase during heat-exposure at 1100 °C were classified into three types: γ matrix→σ→μ, γ matrix→P→μ, and γ matrix→σ→P→μ.

Acknowledgments

This work was funded by National Natural Science Foundation of China (51771148, 52071263, 52031012, 52322410), Science Center for Gas Turbine Project (P2021-A-IV-001-001), The Key Research and Development Program of Shaanxi Province

(2023-YBGY-432), Natural Science Basic Research Plan in Shaanxi Province of China (2021JC-13) and Research Fund of the State Key Laboratory of Solidification Processing (NPU), China (2021-QZ-03).

Conflicts of interest:

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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