THE STRUCTURE OF THE $\gamma'$-PHASE IN NICKEL-BASE SUPERALLOYS

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ABSTRACT

Present day nickel-base superalloys are hardened in part by the precipitation of a phase which has variously been identified as Ni$_3$Al, Ni$_{3}(Al, Ti)$ and $\gamma'$. X-ray diffraction techniques which include precision lattice parameter measurements, intensity measurements, and phase identification are used to define the structural and chemical relationships upon which this phase is based.

These relationships are developed from the following considerations: crystal chemistry and atomic size factors which relate binary Cu$_3$Au-type Ta$_B$ phases (e.g., Ni$_3$Al) and ternary Perovskite-type T$_2$B$_C$$_2$ carbide phases (e.g., Y$_2$AlC), the determination of the number and kind of atoms in the unit cell of Ni$_3$Al and certain ternary phases, the crystallographic relationship between the structure of Y$_2$C and Y$_2$AlC, and phase relations in certain quaternary alloys.

From these considerations it is shown that the $\gamma'$ phase may best be characterized as a Perovskite-type carbide phase having the chemical formula T$_2$B$_C$$_2$. A model of the $\gamma'$ structure is presented which indicates the position of the various atomic constituents based upon whether they are T or B elements. (An atomic component is considered of the T type if it is capable of substituting for nickel in Ni$_3$Al, of the B type if it can replace the aluminum. The essential features of this model are: T and B elements form an ordered T$_2$B lattice of the Cu$_3$Au type; carbon atoms are located only in octahedral holes in the centers of the Cu$_3$Au-type cells thereby establishing Perovskite-type T$_2$B$_C$$_2$ unit cells; the effective size of T and B atoms in the T$_2$B$_C$$_2$ unit cell is the same; hyperstoichiometric alloys, (ratio of B atoms to T atoms greater than one) will contain B atoms at face-centered positions in addition to a small amount of equilibrium vacant sites; in all alloys aluminum will preferentially occupy the cube corners of the unit cell; the amount of carbon which is soluble in T$_2$B$_C$$_2$ at any particular temperature is determined both by the distribution of the elements which are carbide-formers and the elements manganese, iron and cobalt. This model accounts for microstructural changes which occur in some nickel-base superalloys as a function of temperature and composition.

INTRODUCTION

The strength of present day nickel-base superalloys at high temperature is attributed in part to the presence of a dispersed phase ($\gamma'$) in a solid solution matrix. The properties of these superalloys may be changed by modifying the gross composition so as to alter the relative amounts of the dispersed phase, the matrix, and the small amount of carbide phases which are present. Undoubtedly, these modifications also change the composition of these various phases and this change also greatly affects the properties of the alloys. Nevertheless, very little attention has been given to the composition and arrangement of the elements in the crystal lattice and to the influence of this on the properties of the alloy. It is known for example that crystal irregularities such as those produced by lattice vacancies, interstitial atoms, and substitutional atoms of different sizes greatly effect
mechanical properties. It therefore becomes desirable to investigate these structural features.

The dispersion hardening constituent as it appears in superalloys has variously been identified as Ni₃Al, Ni₃(Al, Ti) and γ'. Where microprobe analysis or other means of analysis have been used to obtain the composition of the γ' phase, the following elements have been detected in concentrations greater than five atom percent: nickel, cobalt, titanium, aluminum, and chromium. It is known that the phase also contains a host of other elements in smaller amounts.

The structure of the stoichiometric binary Ni₃Al phase is of the Cu₃Au type, L1₂ Strukturbericht. A ternary carbide phase has lately been identified that bears a close relationship to the phases of the Cu₃Au type. In conjunction with observations to be made later, this similarity served as an indication that an understanding of the γ' phase might be obtained by characterizing the factors governing the nature and stability of the Ni₃Al and ternary carbide phases. In this paper, therefore, these phases are first characterized, then they are related to the γ' phase, and finally from this information a model of the γ' phase as it appears in superalloys is constructed.

**EXPERIMENTAL**

Alloys weighing about 10 g were prepared by arc-melting powder compacts made from various components on a water-cooled copper hearth using a tungsten electrode in a gettered argon atmosphere. With the exception of the rare earth metals, the purity of the starting materials was better than 99.9%. The purity of the rare earth elements used in this study was 99%. The experimental details have been described elsewhere.¹

**THE UNIT CELL OF Ni₃Al AND T₃BCₓ**

The cubic unit cell of Ni₃Al which is of the Cu₃Au-type structure is shown in Figure 1(a). The aluminum atoms occupy the cube corner positions and the nickel atoms the face-centered positions. The ternary carbide phases which are of interest in this investigation are characterized by the general formula T₃BCₓ (e.g., Co₃AlC₀.₁₁). The x value is calculated by dividing the atom percent of carbon by twenty. The arrangement of the metal atoms in the unit cell is the same as shown in Figure 1(a), the T and B atoms

¹ References are at the end of the paper.

Figure 1. Unit cell of Cu₃Au- and T₃BCₓ-type structures.