SAE The Engineering Society For Advancing Mobility Land Sea Air and Space® INTERNATIONAL
400 Commonwealth Drive, Warrendale, PA 15096-0001

AEROSPACE STANDARD

SAE AS5491

Issued 2000-12

Calculation of Electron Vacancy Number in Superalloys

1. SCOPE:

1.1 Purpose:

This Aerospace Standard establishes a uniform procedure for calculation of electron vacancy numbers in superalloys. It is intended for use by suppliers of raw materials and parts, typically castings, for which control of electron vacancy number is required by the raw material specification.

1.2 Application:

This procedure has been used to estimate the potential for alloy phase instability by calculation of the density of electrons per atom in nickel-based superalloys.

1.3 Background:

1.3.1 Complex, highly alloyed superalloys have been observed, for some alloy chemistries and under certain conditions, to form precipitated phases which can adversely affect strength and ductility. These phases, typically of a crystalline structure known as topologically close-packed, or TCP, appear after extended exposure at temperatures in the range from 1300 to 1650 °F (704 to 899 °C). Such phases include sigma (σ), mu (μ) or Laves. Their tendency to precipitate from the alloy matrix has been related by researchers such as Boesch and Slaney (See 4.1) and Woodyatt, et al. (See 4.2) to the density of electrons per atom as expressed by the electron vacancy number N_v, as shown in Equation 1, as follows:

$$N_v = \sum_{i=1}^{n} m_i (N_v)_i \quad \text{(Eq. 1)}$$

1.3.1 (Continued):

where:

N_v is the electron vacancy number for the alloy
m_i is the atomic mass fraction of the ith element in the alloy composition, and
$(N_v)_i$ is the electron vacancy number of the ith element.

Determination of the electron vacancy concentration requires an understanding of the phases which precipitate in superalloys as well as the sequence in which they form in the gamma matrix. In general, this sequence is (a) the precipitation of borides, (b) the precipitation of carbides, and (c) the formation of gamma prime. When these phase reactions are considered, and adjustments made to the composition to take them into account, the residual matrix composition may be determined. From that residual matrix the electron vacancy number is then calculated.

1.3.2 The sequence of precipitation of strengthening phases is addressed as follows:

1.3.2.1 Nickel, chromium, titanium and molybdenum form a boride as $(Mo_{0.5}, Ti_{0.15}, Cr_{0.25}, Ni_{0.10})_3B_2$.

1.3.2.2 All carbon is assumed to form carbides of the type MC and $M_{23}C_6$. It is assumed that MC carbides take half the carbon, reacting in sequence with tantalum, columbium, zirconium, titanium and vanadium. The remaining carbon then reacts with chromium, molybdenum and tungsten to form $Cr_{21}(Mo,W)_2C_6$.

1.3.2.3 Gamma prime is formed from the remaining aluminum, titanium, hafnium and columbium and 3 percent of the original amount of chromium by combining with three times that total in nickel, i.e., $Ni_3(Al, Ti, Cb, Hf, Cr)$.

1.3.2.4 The remaining chromium content is adjusted for that lost due to formation of borides, carbides and gamma prime.

1.3.2.5 The remaining nickel content is adjusted for that tied up in boride and gamma prime formation.

2. APPLICABLE DOCUMENTS:

None.

3. TECHNICAL REQUIREMENTS:

3.1 Calculation of N_v:

3.1.1 N_v will be calculated in the following order:

3.1.1.1 Conversion of weight percentage to atomic percentage for each element

3.1.1.2 Calculation of boron and carbide precipitation

3.1.1.3 Calculation of gamma prime precipitation

3.1.1.4 Calculation of the residual gamma matrix composition

3.1.1.5 Determination of electron vacancy number, N_v

3.1.2 It may be helpful to set up a matrix similar to Table 1 to facilitate recording compositions through the process of electron vacancy number calculation.

3.2 Conversion to Atomic Fraction:

3.2.1 Enter in column A the weight percent of the individual elements by row. When the weight percent is unknown, or the element is not found in the alloy, enter zero (0). The weight percent of nickel is determined by adding the percentages of the other elements and subtracting the sum from 100.

3.2.2 Divide the weight percent of each element (the entries in column A) by their respective atomic weights (from column B) and enter this value in column C in the table. Sum the entries in column C; then individually divide the entries for each element in column C by the sum of column C. Enter this value in column D. This is the atomic fraction of that element.

3.3 Calculation of Phase Precipitations:

For the next series of calculations, reference will be made to cell locations in the table, such that D1 refers to the value of the entry in column D, row 1 (i.e., the atomic fraction chromium) and E5 is the residual matrix atomic percent of cobalt, adjusted for precipitation of second phases.

3.4 Boride and Carbide Precipitation:

3.4.1 Chromium: Multiply D1 by 0.97 and subtract the quantity [(0.75)(D6) + (1.75)D8)], where:

D1 is the atomic fraction of Cr
D6 is the atomic fraction of B
D8 is the atomic fraction of C

Enter the result in E1.

3.4.2 Molybdenum: From D3, subtract the quantity {[(0.75)(D6) + (0.167)[(D8)(D3)/(D3+D14)}, where:

D3 is the atomic fraction of Mo
D6 is the atomic fraction of B
D8 is the atomic fraction of C
D14 is the atomic fraction of W

Enter the result in E3.

3.5 Gamma Prime Precipitation:

3.5.1 Nickel: Add (0.525)(D6) to D19. Subtract from that sum the following quantity: 3[(D4)+(0.03)(D1) + D16 + D2 + D15 – (0.5)(D8) + (0.5)(D13) + D17], where:

D19 is the atomic fraction of Ni
D6 is the atomic fraction of B
D4 is the atomic fraction of Al
D1 is the atomic fraction of Cr
D16 is the atomic fraction of Cb
D2 is the atomic fraction of Ti
D15 is the atomic fraction of Ta
D8 is the atomic fraction of C
D13 is the atomic fraction of V
D17 is the atomic fraction of Hf

Enter the result in E19

3.5.2 Vanadium: Enter (0.5)(D13) in E13, where D13 is the atomic fraction of V.

3.5.3 Tungsten: From D14, subtract the quantity [(0.167){(D8)(D14)/(D3+D14)}], where:

D14 is the atomic fraction of W
D8 is the atomic fraction of C
D3 is the atomic fraction of Mo

Enter the result in E14

3.5.4 Enter zero (0) in E2, E4, E6, E8, E15, E16, and E17.

3.5.5 Enter the value found in D5, D7, D9, D10, D11, D12, and D18 in the corresponding rows in column E.

3.6 Calculation of the Residual Matrix Composition:

3.6.1 Sum the values in column E, and enter at the bottom of column E.

3.6.2 Column F is the matrix atomic fractions. For each row, divide the value in column E by the sum of column E calculated in 3.6.1.

3.7 Calculation of Electron Vacancy Number:

3.7.1 Multiply the matrix atomic fraction in column F by the individual elemental electron vacancy numbers in column G, and enter the product in the corresponding row in column H.